Heterogeneity in Agent-Based Models

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Abstract

Agent-based models are an incredibly flexible tool that among other things, allow modellers to capture heterogeneity in agent attributes, characteristics, and behaviours. This study defines heterogeneity in agent-based models as agent granularity: the level of description used to define the agent population. Consequently, this increased complexity can make the already challenging tasks of calibration and parameter identification, even more difficult. Although modellers recognise the significance of model calibration, the process of uniquely determining model input from any given model output is overlooked. This thesis proposes an impact of heterogeneity in agent-based models is parameter non-identification.

To this end, this research conducts a thorough examination of agent heterogeneity by the comparative study of homogeneous and heterogeneous scenarios in agent-based models. Using an emotional contagion case study model and approximate Bayesian computation calibration, it finds that the introduction of heterogeneity results in inaccurate parameter calibration compared to the homogeneous case. This study proposes the inaccurate results as the consequence of a failure to uniquely distinguish the effect of additional parameters in the model. Furthermore, failing to identify model parameters limits the predictive or forecasting power of the agent-based model. A simple case study is used to demonstrate that the use of unidentifiable models to inform realworld governmental and social policies can lead to erroneous conclusions and potentially unsound interventions.

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Abbreviations

ABC	Approximate Bayesian Computa-	ABC-SMC	Approximate Bayesian Computa-
	tion		tion Sequential Monte Carlo
ABMs	Agent-Based Models	ACE	Agent-Based Computational Eco-
			nomics
ARE	Average Relative Estimation Error	BDI	Belief-Desire-Intent
CA	Cellular Automata	DMC-RPA	Diverse Model Calibration for Ro-
			bust Policy Analysis
FIM	Fisher Information Matrix	GIS	Geographic Information Systems
HAM	Heterogeneous-Agent Models	MAP	Maximum a Posteriori Probability
MC	Monte Carlo	MCMC	Markov Chain Monte Carlo
MCSUI	Multi-City Study of Urban Inequal-	ODD	Overview, Design Concepts and
	ity		Details
ODE	Ordinary Differential Equations	RMSE	Root Mean Square Error
SEIR	Susceptible-Exposed-Infectious-	SEIS	Susceptible-Exposed-Infectious-
	Recovered		Susceptible
SIR	Susceptible-Infectious-Recovered	SIS	Susceptible-Infectious-Susceptible
SISa	Susceptible-Infectious-Susceptible-	SOSa	Susceptible-Optimistic-
	Spontaneous		Susceptible-Spontaneous
SPSa	Susceptible-Pessimistic-		
	Susceptible-Spontaneous		

Chapter 1

Introduction

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1.1 Research Motivation

Agent-based models (ABMs) are an exemplary tool, well-known for their use in analysing the inherent and intricate complexities of many systems (Buchmann, Grossmann, and Schwarz 2016). They can uncover system patterns and characteristics of large-scale hierarchical structures from simple individual-level processes. Choosing to simulate a system with ABMs has its advantages, but there are two main attractions: (1) capturing the heterogeneity of agent attributes and, (2) creating a network of interactions (Bonabeau 2002). In this study, heterogeneity refers to the concept of agent granularity but this idea will be explored further in Chapter 2. Modelling a system heterogeneously oftentimes enriches the understanding and interpretability of the system dynamics; it connects attributes to observed behaviours and then to model outcomes. The insights gathered from connecting these facets may uncover incredibly valuable information about the system's dynamics that may have otherwise remained unknown (Reeves et al. 2022). Capturing heterogeneity allows the modeller to simulate various behaviours directly reflecting the target system. On a micro-scale, agents interact and form relationships with each other and their shared environment; on a macro-scale, this creates a network of interactions.

Researchers have applied ABMs to the study of biological (Politopoulos 2007; An et al. 2009), social (Epstein and Axtell 1996; Gilbert and Terna 2000; Conte and Paolucci 2014), physical (Torrens 2010; Heppenstall, Crooks, See, et al. 2012; Zhu et al. 2013) and economic (Tesfatsion 2002; LeBaron 2006; Arifovic and Duffy 2018) phenomena, with the hopes of explaining the connection between individual behaviours and aggregate outcomes. Nonetheless, the application and scope of ABMs are not limited to the above; they are a tremendously pliable tool with an exhaustive list of actual and potential applications. For example, one of the earliest ABMs was created by Schelling (1971) which aimed to describe segregation as an emergent behaviour. Using a few parameters Schelling-Sakoda demonstrated how segregated neighbourhoods might emerge as the result of individual decision rules. These decision rules were ultimately governed by a preference to reside with neighbours which they considered similar. More recently, Gatti and Desiderio (2015) created a macroeconomic model addressing monetary policy; in the model, consumers and prices changed according to simple expectations. From the simple rules, they were able to reproduce business cycles similar to those observed in real life. With ABMs it is possible to define and display various characteristics and behavioural types through agents, these types of models are referred to as heterogeneous. Although ABMs can accommodate the differences in agent attributes and behaviours, they also allow for the study of systems that assume uniformity, these types of models are referred to as homogeneous. The flexibility of ABMs provides modellers with the choice to produce aggregate or individual outcomes, but even aggregate results can be examined on a micro-scale; unlike other methods, such as differential equations, that assume homogeneity in agent attributes and can only be evaluated aggregately.

Nevertheless, the choice between assuming homogeneity or heterogeneity depends on the modeller's primary objectives and the nature of the real-world system. When choosing underlying assumptions, modellers should always consider the perceived level of detail within the real-world system (e.g. degree of complex individual behaviours, the resolution quality of the environment, etc.) and aim to represent it as accurately as possible. Detail refers more generally to model attributes, both the agent and environment attributes. However, within the constraints of this thesis, detail will refer specifically to the number of agent attributes or agent granularity. Highly granular models are usually characterised by an increasing number of agent parameters, and consequently, these are high-dimensional models. Modellers could also consider the *impact* either assumption may have on the validity of the model. In other words: if the system is modelled adequately when assuming homogeneity, what is the perceived impact of introducing heterogeneity on the model outcomes? Could the model with heterogeneous attributes better capture the dynamics evident in the real-world system?

For example, modelling heterogeneity plays an important role in epidemic modelling and evaluating interventions (Thieme 1985; Mollison 1995; Berestycki et al. 2023). Though modelling COVID-19 homogeneously has been successful (Wang, Zhou, et al. 2022), Ellison (2020) proposes that calibrating the classic epidemic model to data generated by a heterogeneous model of COVID-19, results in biased forecasts and uncertainty. The particular biases identified were the underestimation of how quickly herd immunity is reached, an underestimation of differences across regions, and biased estimates of the impact of endogenous and policy-driven social distancing. Donnat and Holmes (2023) identifies modelling the reproductive number for COVID-19 heterogeneously as paramount in the quantification of the potential scope of the pandemic and the selection of an appropriate course of action. In their study of contact networks, Thomas, Huang, et al. (2020) proposes that uneven population distribution on the spread of the COVID-19 disease, produces dramatic differences in social exposures to those with the illness and increases pressure on health care systems in ways that are not well captured by classic epidemic models (Lu et al. 2021). These studies demonstrate the significance of heterogeneity and the importance of considering its potential impact on model results.

The aim of scientific exploration is explanatory power; the ability to explain and outline relationships, dynamics and interactions. Despite models being typically viewed as a reflection of a system, a more pragmatic approach has been proposed, whereby models are viewed as tools designed for specific purposes. Thus, model performance or model goodness can be assessed against how good it is for its declared purpose (Edmonds et al. 2019).

As computational resources and capabilities have increased in time, modellers might assume the more descriptive a model, through an increasing number of variables, the better its explanatory power. Empirically, however, this may not always prove to be true as the potential to *overfit* will always exist, regardless of the method's structural flexibility.

More specifically with ABMs, the model input could be described as a distribution of initial states and behaviours for each agent and the output would be distributions of what is observable (Wallace and Ogawa 2015). For example, when the correct vector of parameter values is known (from real data), then changing the values could produce different outcomes using the same model structure. Then, if each parameter value can be directly mapped to the distribution of observables one-to-one, then there is parameter identification. But through the introduction of additional parameters, the effect of each parameter value becomes difficult to distinguish therefore harder to map directly to the distribution of observables. The added dimensionality and complexity observed in the model make parameter identification more challenging to achieve.

Now, consider a case where the parameter values are used to simulate the behaviour of different policies, including policies not tried in the original environment. Where each parameter represents a specific policy, then successfully identifying their parameter values means capturing the effect of each parameter on the output, with some certainty. And with this, modellers can consider each policy according to appropriate needs. Regardless of the purpose of the ABM, predictive or explanatory, if parameters are unidentifiable, this indicates that the effects of the model input are indistinguishable. Therefore, full knowledge of parameter values becomes irrelevant and policy suggestions redundant, as the relative strength of each parameter is unknown and cannot be mapped to the distribution of observables. Parameter identification is often overlooked in the process of parameter estimation, as in most cases parameter values are known from real data, so identifying the effect of each input from the output seems futile.

But as with the dangers of overfitting, it is possible that the more heterogeneous the model, the greater the potential for parameter non-identification. This problem serves as motivation for this

thesis which proposes parameter identification issues as an impact of heterogeneity in ABMs. This thesis will use a case study of emotional contagion, which should be considered as a toy model for demonstrative purposes, to present the problem of parameter identification as an impact of heterogeneity. This study considers the variety of ways that heterogeneity features in ABMs, and hence concludes that an all-inclusive precise definition is unfeasible. Thus, this study proposes heterogeneity refers specifically to agent granularity. Agent granularity indicates the coarseness of descriptive attributes and behaviours assigned to the agent population. Typically, the more descriptive an ABM, the more parameters are included in the model. Therefore, this study proposes that the impact of creating increasingly descriptive models can lead to parameter identification issues. This is demonstrated in the calibration of a case study model, where the introduction of heterogeneity is shown to negatively impact the accuracy of parameter calibration. Though this study is successful in highlighting the impact of heterogeneity, it highlights the following: the critical need for an established method which examines the identification of parameters in ABMs. As will be proposed in this investigation, the process of calibration and identification cannot be separated, hence ABM calibration methods should aim to integrate indicators that represent how well ABM input (i.e., distribution of initial states) maps directly to the ABM output (i.e., distribution of observables).

1.2 Aims and Objectives

The overarching aim of this thesis is to investigate the impact of heterogeneity on the parameter identification of agent-based models. To achieve this, the following objectives were formalised:

- Review and discuss the literature related to ABMs, with a focus on heterogeneity as a characteristic. Also, briefly review the literature on emotional contagion and compartmental models to facilitate the design and development of the case study model.
- 2. Design and build the case study ABM, simulating the transmission and infectiousness of emotional contagion. Then determine optimal values for the ABM using sensitivity analysis.
- 3. Evaluate the ABM by assessing its response to varying parameter values using calibration

to examine the parameter space.

4. Define and investigate the problem of parameter identification in heterogeneous ABMs.

1.3 Main Contributions

The section summarises the main contributions of this thesis in the following points:

- This thesis proposes a specific definition of heterogeneity in ABMs for which its impact can be measured. Heterogeneity is limited to the agent component and is defined as agent granularity; which refers to the coarseness of descriptive attributes and behaviours assigned in the agent component e.g. the number of model parameters used to describe the agent class.
- This thesis proposes an impact of modelling heterogeneously in ABMs is parameter nonidentification. This study demonstrates the existence of parameter identification issues in heterogeneous ABMs and how they can be detected using approximate Bayesian computation calibration.
- 3. Parameter identification i.e. the ability to identify a unique set of parameter values that produce a particular model output, should be included in the standard ABM calibration process. This thesis proposes: that to successfully calibrate an ABM should go beyond presenting a single parameter point or capturing uncertainty by presenting a selection of best-fitting parameters, and go a step further by uniquely distinguishing the model input from the given output.

1.4 Thesis Structure

This section presents the structure of this thesis.

Chapter 2 introduces ABMs and outlines their characteristics and methodology. It begins with an introduction to complex systems and computational models. The chapter then presents ABMs, highlighting their components, features and characteristics. To conclude, the chapter discusses relevant literature illustrating the impact of agent heterogeneity.

Chapter 3 extends the literature review to the study of emotional contagion and compartmental models. The purpose of this review is to frame the design and development of the case study model.

Informed by the previous chapters, Chapter 4 outlines the case study model. It describes model construction using the ODD protocol, presenting each element of the emotional contagion model. It includes the results of model exploration to shed some light on the system dynamics. In addition, presents the full results of the sensitivity analysis conducted on the case study model.

Chapter 5 and Chapter 6 are complimentary. Chapter 5 evaluates the case study model using simulated data using approximate Bayesian computation calibration. Although calibration methods are typically used to validate models, Chapter 6 will use them as tools to introduce parameter identification in ABMs.

Finally, Chapter 7 concludes this study with a summary, critical reflection and suggestions for future research.

Chapter 2

Agent-Based Models

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2.1 Chapter Overview

This chapter will provide a brief overview of Agent-based models (ABMs). It begins in Section 2.2, by outlining the challenge in modelling complex systems and subsequently presents suitable computational approaches, including ABMs in Section 2.3. To consider its potential application, Section 2.4 highlights the standard ABMs components, features and characteristics and also presents capturing heterogeneity as a key advantage. Finally, Section 2.5 evaluates agent heterogeneity further, first by offering a definition and second by undertaking a comparative study of homogeneous and heterogeneous scenarios in ABM literature to assess the impact of modelling heterogeneity. This section presents the following observations: *i* agent heterogeneity is often displayed in two

non-mutually exclusive forms: the categorisation and/or variability of the agent population and attributes, *ii*) agent heterogeneity is extrinsic, in that heterogeneity is initialised into a model but the evolution away from the initial heterogeneity is rarely monitored. Heterogeneity which develops outside of the initial conditions is referred to as generated heterogeneity, *iii*) the variable used to demonstrate agent heterogeneity can impact model results, iv) undetected pre-conditions between components can affect the impact of agent heterogeneity, v) the object of study and research purpose are contributing factors to deciding between imploring homogeneous or heterogeneous assumptions, vi) If agent interactions generate network effects, then the types and effects of heterogeneity found in network sciences apply to agent-based models. Two types of heterogeneity found in network sciences are structural and relational heterogeneity. Structural refers to the different structural changes that arise as a direct result of agent heterogeneity; relational heterogeneity emerges directly from agent interactions and finally, vii) Comparative homogeneous and heterogeneous scenarios should be a standard, to help evaluate the impact heterogeneity has on the system being modelled. Modelling heterogeneity may be a computationally expensive task, but in some cases has been made unnecessarily so; thus it is important to discern when the increased granularity no longer enriches the model's explanatory or predictive powers.

2.2 Complex Systems

Complex systems are systems that are difficult to model as a result of the inherent dependencies, relationships and interactions between their parts or their environment (Bar-Yam 2002). To investigate any system, animate (i.e., living organisms) or inanimate (i.e., lifeless objects), learning what they are comprised of is an important initial step (Sterman 1994). Although identifying each part or component is essential, studying them individually is an impractical task as the more complex a system, the more components (Hmelo-Silver and Azevedo 2006). The deeper the investigation goes, the more complex the system gets and the harder it becomes to piece each component back together. Each component is rich and has depth, this is why researchers dedicate their whole careers to the understanding of one area (Newman 2011).

An example of this is the study of Sciences which has three broad branches: formal sciences,

natural sciences and social sciences. If these branches are considered as components, they can be broken down further into sub-components e.g., natural sciences is the study of natural phenomena, this includes biology, physics, chemistry, cosmology and geology. Again, these sub-components can be broken down even further. By focusing on individual components of a system in complete isolation, science has made great progress (Wimsatt 2006). This approach is known as reductionism, which implies that a system is no more than the sum of its parts (Kricheldorf 2016). However, in instances where interactions are present in systems, this strategy falls short by ignoring the value of each connection present in the system.

Hence, to effectively study a complex system is to investigate the relationship and interactions between the individual components, the whole system and the environment (Arthur 1993; Gell-Mann 1995). The object of study is the collective behaviours that emerge from each component, which may differ in terms of characteristics, properties and behaviours (Fisher and Pruitt 2020). The challenge then lies in identifying an appropriate methodology that captures interactions such as non-linearity, spontaneous order, adaption, feedback loops and emergence sufficiently (Flake 2008; Mitchell 2011).

To confront this challenge, researchers propose computational models as an appropriate approach to modelling complexity (Schweber and Wächter 2000). The following section will present some computational methodologies.

2.3 Computational Models

Computational models are simulations that act to represent the processes and interactions which standardly comprise a system (NIH 2020). Computational models can take the form of simplified mathematical expressions (Li, Ban, et al. 2018), but can also describe linear and nonlinear complex systems (Grubb et al. 2020) where intuitive analytical solutions are not readily available. These types of computational models simulate various experiments with the model by adjusting the parameters of the system and studying the differences in the outcome of the experiments (Ben Youssef 2016). The computational methodology approach is widely used across disciplines, from physics and engineering (Oberkampf, Trucano, and Hirsch 2004; Schäfer and Schäfer 2006; Liu, Feng,

et al. 2022; Omelchenko et al. 2023), mathematics (Stoer 2006; Akin 2014) to psychology and cognitive sciences (Fodor 2000; Sun 2008; Palminteri, Wyart, and Koechlin 2017; Putnam 2018). There is no argument against the key contributions computational methods have made toward understanding the intricacies and dynamics of complex systems, across disciplines and specialities from public policy to autonomous systems (Calder et al. 2018).

There is a wide range of computational models frequently implored in the study of complex systems. The choice of which to use depends on the underlying assumptions and abstractions about the target system. The main types of computational models are now reviewed in brief:

- **Deterministic models** produce the same outcome on multiple runs with the same inputs. There is no randomness or spontaneity in these models. Determinism allows for absolute assertions which can be incredibly valuable. However, it is important to consider whether determinism is evident in the target system first before implementation.
- Non-deterministic models produce different outputs on different runs, even when the inputs are the same. They do not specify a path of execution, thus any behaviours observed as an outcome could present in any number of ways.
- Static models have outputs that do not vary or change over time. Model input is studied in isolation with no concept of time. An example of this is spreadsheets with no time explicitly encoded as an input.
- **Dynamic models** have outputs that do vary or change over time. Some examples of dynamic models are ordinary and partial differential equations (Ockendon et al. 2003; Witelski and Bowen 2015), they represent the rate of change over time and are used in areas including, finance, economics and engineering. Similarly, system dynamics (Forrester 1968) uses ordinary differential equations to explore the possible effects of different scenarios to unveil some unanticipated consequences; they are a useful tool to discover structural changes in behavioural patterns.
- **Discrete models** use values that increase in steps (i.e., a series of integers) to represent objects or events. An example of discrete models is transition systems which are based on

the observation of a set of discrete states (Keller 1976).

- **Continuous models** observe events which could occur at any point in time, they often use real numbers and can be visualised as 'smooth' or 'dense'. Differential equations are an example of continuous models.
- Stochastic models (Pinsky and Karlin 2010) or probabilistic models have an inherent element of random, or uncertain, behaviour and the events are assigned probabilities. This can be viewed as a special case of a non-deterministic model in which the probabilities are known.
- Individual-based models follow individuals through a system, tracking changes to behaviour and their interactions. Together individuals form a complex and emergent system, and individual behaviours cannot be derived from simple aggregation. Agent-based models (Gilbert 2019) are an example of individual-based models and have been used to model social insects, telecommunications networks and stock markets.
- **Population models** represent large groups of homogeneous individuals. Population models can also model individuals with attributes that vary on a small scale based on counterabstraction (Pnueli, Xu, and Zuck 2002), which records the number of individuals with each trait.
- Logic models are descriptions or statements which outline a chain of cause and effect which have led to the desired outcome. Formal logic models range from classical predicate logic (Kleene 2002), to temporal logic (Fisher 2011) for future behaviours, and probabilistic temporal logic (Hansson and Jonsson 1994) for future certainties and uncertainties.
- Automata and process algebraic models (Baeten 2005; Milner 2009) are simple representations of concurrent events. These models follow algebraic laws to define how operators relate to each other.
- Black-box models are machine learning devices which fit data and trends without revealing internal workings. Machine learning (Murphy 2012) uses algorithms to learn from the past, data and experience. These models are useful where there is little knowledge about how the

system works, but where data is available.

Each of these computational models has its advantages and disadvantages. The choice of model is often based on the system dynamics, theoretical assumptions or researcher expertise. This thesis proposes ABMs as a sufficient computational approach to simulating complex systems, particularly where the complex systems are comprised of heterogeneous components. The following section will present ABMs in detail and evaluate their suitability for modelling heterogeneity.

2.4 Agent-Based Models

The previous section briefly presented a variety of computational models commonly used to study complex systems. This thesis will consider a particular type, namely individual-based models or agent-based models (ABMs). Agent-based modelling may not have a long history but extensive contributions have been made across many disciplines (Heath, Hill, and Ciarallo 2009). Its widespread use is accredited to the ability to simulate theories, particularly in cases where data is unavailable (Abdou, Gilbert, and Tyler 2008), but there are numerous characteristics and unique features which modellers consider to be incredibly beneficial.

ABMs are an immensely powerful tool used to model systems containing a collection of autonomous decision-making entities called agents. Each agent assesses their circumstances and relationships before making decisions based on a set of governing rules (Bonabeau 2002). As a result, agents can display a range of behaviours given the dynamics of the system. This is referred to as a "bottom-up approach" i.e., the development and growth of whole systems from individual interactions (Epstein and Axtell 1996). Crucially, the bottom-up approach gives rise to emergent phenomena, even in the simplest ABMs (Reynolds 1987). As mentioned previously, there is a great deal of valuable insight that can be extracted from modelling complex systems, which ABMs can provide. Further, the evolution of agents and their environments allows for the unpredictable to emerge. More sophisticated ABMs, tend to be less abstract and incorporate more detailed representations of the real world (Zhang, Valencia, and Chang 2021).

The earliest and most recognised historical influence on the development of ABMs is Cellular

Automata (CA) (Wolfram 1983). CA is defined as "discrete spatiotemporal dynamic systems based on local rules" (Miller 2009) and are considered the simplest framework for modelling complex systems (Clarke 2014). CA are usually one- or two-dimensional lattices (Janssen 2005). They have simple rules which generate complex behaviour; these rules describe the cell state for t + 1by first considering the neighbouring cell states, where time is t and t = 0, 1, 2, ..., n. In their simplest form, cells are represented with binary states (0 or 1) (Wolfram 1983). CA is an established methodology in its own right and has seen considerable application due to its simplistic nature. However, this same advantage of simplicity can be considered a disadvantage. CA only uses a few rules to update cell state depending on neighbourhood states and therefore has limited application. Some complex behaviours do not depend solely on the neighbourhood but on internal factors. So, to model more realistic situations agents need extensive capabilities more than CA provides. Having said that, determining an appropriate methodology for research should always consider the type of complexity the system possesses.

Following CA came Schelling-Sakoda-Sakoda's Segregation Model (Schelling 1971), which is widely accepted as the first agent-based model (Hatna and Benenson 2012). The model had two main features: *i*) cells which represented residences in urban areas and, *ii*) two types of agents which populated those areas. Throughout the simulation, agents would move residences based on a satisfaction value they derived. This resulted in the clustering of the same types of agents within the same neighbourhoods. In comparison to CA, Schelling-Sakoda's model produced complex behaviours which considered the environment and internal factors (i.e., the satisfaction or comfort threshold values) which more naturally emulated the dynamics of the residential segregation of ethnic groups in real life. The segregation model embodied what is now considered fundamental features of ABMs: agent autonomy, emergent phenomenon, a shared environment and interactions.

The advantages of ABMs can be summarised as: *i*) ABMs can capture emergent phenomena, *ii*) ABMs are a "natural" descriptor of systems and, *iii*) ABMs are agile and incredibly flexible.

Emergent phenomena are the observed result of interactions between individual entities, it is the outcome of the system as a whole (Bonabeau 2002). An emergent phenomenon can have properties dissimilar to the system's individual parts, i.e. a traffic jam moves in the opposite direction to

the vehicles that give rise to it. Additionally, when the investigation of individual behaviour is essential, ABMs incorporate the use of thresholds and if-then rules. Individual behaviours may also exhibit memory, path-dependence, learning and adaption and many other features that effectively introduce heterogeneity (Bazghandi 2012).

Moreover, ABMs are natural descriptors of behavioural entities; from describing traffic jams, and financial markets to simpler mechanisms such as people walking through exits, ABMs make it possible to model reality closely (Eberlen, Scholz, and Gagliolo 2017). For example, in crowd management studies with the aim of calculating the density of people in an area, it is more natural to describe how people walk through doorways than to use equations. This is because density equations only produce aggregate results of behaviours shown, whereas the agent-based model approach enables the modeller to examine both aggregate and individual behaviours. Therefore, ABMs are a great tool for modelling multi-scale systems and processes.

Lastly, flexibility refers to the adaptability of the ABM framework: the structure of an ABM allows for the easy adjustment of model parameters according to the objective (Grimm, Berger, Bastiansen, et al. 2006).

To summarise, this subsection provides an overview of ABMs. It introduces ABMs as a concept, and then briefly outlines their history and influences. The following subsections will explore the key features, characteristics and components which typically comprise ABMs.

2.4.1 Components, Features and Characteristics

There are three key components to any agent-based model: (1) agents, (2) their environment and, (3) governing rules, behaviours and relationships. These components are visualised in Figure 2.1, which illustrates an agent population attributed with a list of descriptive features. The environment is the encompassing system in which the agents exist and varies from spatially to abstract constructs (e.g., network structures, grid cells or attribute measures). Agents' behaviours are determined by governing rules which determine how agents interact and form relationships (Macal and North 2005; Abdou, Hamill, and Gilbert 2012). ABMs are fairly simple to implement, they rarely have complicated architectures and designs but can accommodate complexities.

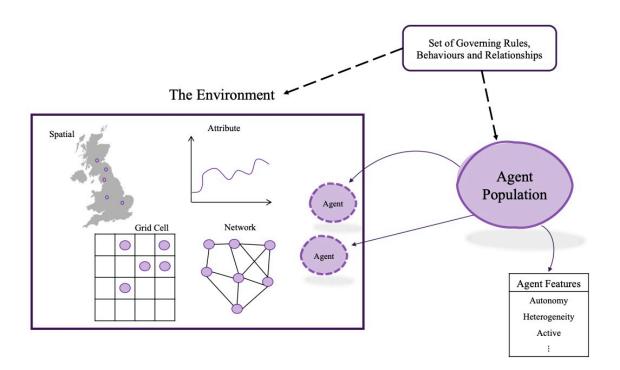


Figure 2.1: The Agent-Based Model Framework

Now, depending on research objectives, disciplines and applications, these components are adjustable and can be computed to suit specific purposes. For this reason, it would be a challenge to list every potential characteristic a model could have. However, there is some agreement on the basic characteristics of each component.

As previously mentioned, agents are a collection of autonomous decision-making entities. Agents can be animate or inanimate, they can take any form from insects and humans to buildings, water droplets and cars (Heppenstall, Crooks, See, et al. 2012). Some modellers class any type of singular component, whether it be software, model or individual, as an agent (Bonabeau 2002). Although there is no universal definition for an agent, some consider agents to have the following characteristics:

• Autonomy: Agents are self-governed, they fulfil their own interests without the influence of any centralised control (Jennings 2000). Agents can freely interact, consume and exchange

information with others and the shared environment and make decisions independently of each other (Wellman 2016).

- Heterogeneity: Agents can differ individually in their preferences, according to their own rules of action (Gilbert 2008). When modelling human attributes, each agent may have an age, sexual orientation, socio-economic status, etc. Agents need not be identical but can be if preferred. Agent groups can be generated from initialisation, but in time agents can form groups organically (Castle and Crooks 2006). Within the scope of this research, heterogeneity will refer to agent granularity, which is the coarseness of descriptive attributes and behaviours assigned in the agent component (Gao, Song, and Wang 2013). The more detailed or granular agent attributes, the more heterogeneous; the coarser agent attributes, the less heterogeneous agents are considered.
- Actions: Agents have full autonomy and are considered active as they can all influence the outcome individually. Active agents tend to have the following features, but are not limited to them:
 - Goal-orientated or Pro-active: This refers to agent behaviour being influenced by the instruction to achieve particular goals (Deadman and Gimblett 1994).
 - Bounded Rationality: The rational-choice paradigm assumes agents are perfectly rational with unlimited access to information and infinite analytical ability (Simon 2000).
 Whereas bounded rationality places limits on agent knowledge and information, this allows them to be inductive and adaptive (Parker et al. 2003).
 - Mobility: Agents can move freely within an allocated space or be static. The type of movement agents display would be dependent on the research objectives.
 - Adaptation or Evolution: Modellers can design agents to 'learn' and make informed decisions from memory. Agent's learning can occur on both an individual or aggregate level, which changes the initial rules for behaviour (Casti 1997).
 - Interactive: Agents can choose to interact amongst themselves and with their environment.

It is important to note that agent characteristics and features are not limited to the ones outlined above, they can be further customised in line with the research objectives and application.

As illustrated in Figure 2.1, agents can have a selection of features and characteristics. The space in which agents exist and exhibit these features is known as their *environment*. Environments can be spatial or abstract. A spatial environment could take the form of a geometrical space, where agents have specific coordinates or locations. The distance between agents is then captured in the continuous space by adjacency for grid cells or by connectivity in social networks (Heppenstall, Crooks, See, et al. 2012). Abstract environments include spaces where agents are static, but information regarding their behaviour and interactions can be captured numerically and visualised in a time series or frequency distribution. Abstract environments are for models in which the location is nonessential. ABM's pliability allows for scenario-based experimentation, where variables and the environment can be controlled, adjusted and then observed. When investigating multi-layer and multi-dimensional system processes, ABMs methodology is flexible enough to capture the dynamics (Brown 2006).

As mentioned above agents are self-governing, meaning they act according to a set of rules that determine their behaviour, how they interact and form relationships. Rules are designed by modellers and can be informed directly from expertise, extracted from published literature or as the result of some numerical analysis. Agent behaviours can range from the simple, reactive "if-then" rules to incorporating standard behavioural frameworks, a popular example being the Belief-Desire-Intent (BDI) model (Macal and North 2008). Behaviours can also be more intricately determined by some artificial intelligence or machine learning algorithms. This also allows for the scheduling of behaviours to occur synchronously or asynchronously. Furthermore, rules can apply to specific groups of agents, ranging in size from the entire population down to a single agent, or can be hierarchical, where layers of rules may apply to smaller subsets of agents. Rules can ensure agents achieve an outlined goal or make them act in complete ignorance of others (Malleson, Heppenstall, and See 2010). But if directed to, agents can interact with each other and their environment and form relationships. Agents can form relationships to help achieve a goal or relationships can be formed as the result of actions; as with the other components, the type of rules,

behaviours and relationships modellers choose to incorporate must consider their specific objective and application.

Agent-based modelling has been used to successfully emulate some real-life complexities. ABMs have been used to investigate molecular systems in biology to better understand the pathways of health and disease (Soheilypour and Mofrad 2018), simulate cancer growth (Wang, Butner, et al. 2015) and bacterial populations (Gorochowski et al. 2012). ABMs have also been applied to translational systems biology, which simulates drug and device design, clinical trials, and drug effectiveness eventually to predict the effects of drugs on individuals (An et al. 2009). In ecology, ABMs have been used to model habitats to better preserve and manage them (McLane et al. 2011), the impact of human disturbances on wildlife (Bennett et al. 2009) and animal behaviour (Tang and Bennett 2010). In social sciences, ABMs have simulated the impact of social influence (Axelrod 1980) and collective behaviour (Epstein and Axtell 1996). In economics and finance, ABMs have explored stochastic volatility on the pricing dynamics of assets (Franke and Westerhoff 2012) and following the 2009 financial crisis ABMs have evaluated the impact warning signals of future crises (Buchanan 2009).

ABMs have an extensive list of applications due to their multitude of advantages. Be that as it may, as with any tool, agent-based modelling has its limitations. When modelling a phenomenon, it is critical to ensure the ABM includes the optimal amount of detail required for the model to serve its purpose (Couclelis 2000). This remains a difficult criterion to satisfy, specifically in systems where there do not yet exist adequate methods to collect data. Although the world has become more data-centric, the availability and accessibility to quality data which appropriately describe real-world systems remain challenging to obtain and fully understand. This introduces further challenges in validating and calibrating the model all of which limit its explanatory power. Nonetheless, computational tools increase the utility of simulation models through customisation and subsequent analysis to meet the requirements of the modeller (Parker et al. 2003).

ABMs facilitate the investigation of whole systems from the bottom up, which means considering individual components in significant detail. It is important then to evaluate model results systematically in the form of sensitivity analysis. To ensure the model results are appropriately interpreted, the modellers must have a robust understanding of the results; typically this would involve varying the initial conditions or model parameters (Axtell 2000). Assessing the model's robustness can be a computationally extensive and time-consuming task. Yet as computing power increases, notably through the utilisation of tools like high-performance computing, model evaluation for large systems can still pose a challenge.

Finally, the replicability of ABMs is rare and is seen as a difficult task. Replication involves the careful examination of models and facilitates robustness analysis which results in increased model reliability and increased literature supporting the observed output (Easterbrook 2014; Thiele and Grimm 2015). Replication and the reuse of models would make a significant contribution to ABMs, but model complexity complicates the task. To overcome this challenge, ABMs should be published with clear documentation and source code. Even though there exist excellent frameworks, such as the ODD protocol to help facilitate this, published models often lack the required detail (Rollins et al. 2014; Thiele and Grimm 2015; Donkin et al. 2017). Despite these limitations, ABMs continue to grow in popularity and remain a useful tool for exploring complex systems. However, there remains notable work to address these limitations and strengthen the agent-based modelling methodology.

2.5 Heterogeneity in Agent-Based Models

The previous section introduced ABMs by outlining their key features and characteristics. One of the main advantages of ABMs is their ability to represent various characteristics (i.e. parameter values, attributes behavioural rules, etc.) through individual agents. This section will begin by briefly discussing the application of ABMs specifically in Economics and Biology, to identify some of the ways heterogeneity has been presented in research. Finally, to investigate the impact of heterogeneity, this section broadly reviews comparative experiments of homogeneous and heterogeneous scenarios in agent-based model literature. Most agent-based model literature does not include comparative scenarios, in turn, the impact of heterogeneity and its significance within those studies are unobservable.

Heterogeneity within the social sciences refers to individual features and attributes that create

differences within populations (Xie 2013). As aforementioned, a prominent feature of ABMs is heterogeneity, which can be used to model individual attributes such as age, gender, and social or health status. The choice of attributes depends on the specific research objectives. Heterogeneity can be presented not only through agents but in their environments and behaviour. Due to this diversity, successfully capturing some attributes in a controlled experiment poses a difficult challenge, most especially when exploring the effects of individual behaviours on a macro-scale. Investigating relationships between individual behaviours and societal macroscopic regularities can be considered the fundamental reason and ultimate motivation for continued research into modelling human behaviour (Epstein and Axtell 1996).

In economics, researchers assume people form rational expectations (Muth 1961). i.e., people will usually make rational decisions assisted by their access to unlimited information and possession of perfect analytical skills. Thus, for a significant amount of time, researchers would only use representative agents in economic models (Nature 2009). A representative agent assumes that all agents are identical, which is a fundamentally untrue assumption to apply when modelling populations. This homogeneous approach to population modelling in economics failed to consider how inherent differences in people greatly impact the decisions they make as consumers. This was highlighted in the wake of the 2007/08 financial crisis, where differences in decision-making and preferences affected the decisions consumers made in the financial markets (Farmer and Foley 2009). However, Tesfatsion (2002) proposed a new methodology for the effective modelling of economic processes called agent-based computational economics (ACE). Rather than modelling agents using the same decision-making process, they allowed agents to choose from a set of possible forecasting strategies. Arthur et al. (1996) created a model where agents could choose from a set of possible forecasting strategies to predict stock prices. They achieved this by assuming agents had bounded rationality i.e. the idea that agents had limited knowledge of market forces. In ACE and heterogeneous-agent models (HAM), heterogeneity is introduced through the bounded rationality assumption and allows for agents to choose their decision-making process from a set of possible strategies. The consequence of this were studies which produced similar dynamics to that observed in real-world financial systems (Hommes 2006; LeBaron 2006; Arifovic and Duffy 2018).

Agent-based modelling in biology has many applications, primarily due to the characteristics listed in the previous section. Specifically when modelling in epidemiology, ABMs can examine the progression of a disease through heterogeneous populations. In ABM models of epidemiology, it is common to include attributes such as health statuses, social networks for contact tracing and spatial/geographical areas. The most important element of modelling epidemics spatially is how the infection spreads (Epstein 2006). Perez and Dragicevic (2009) created an ABM that integrated geographic information systems (GIS) to simulate the spread of measles in an urban environment, as a result of individuals' interactions. They considered the nonlinear behaviour of epidemic spreading by creating a population of agents who were involved in a sequence of heterogeneous stationary and mobile activities. The stationary activities were at fixed locations, such as a home, schools, workplaces, and commercial and shopping areas, whereas the mobile activities included daily commuting activities of individuals through the public transportation system. Moreover Carley et al. (2006) developed a multi-agent network numerical model which was used to simulate the malicious dispersion of 62 diseases. An interesting agent attribute they included was a display of symptoms, they ensured that not every agent with the same disease presented the same symptoms. In epidemic ABMs, to model the spread of diseases means to model agent interactions; not only with each other but with their environment. Therefore, heterogeneity can be represented in both agent individual attributes (i.e., socio-demographic factors, health statuses, symptoms, social network, etc.) but is also presented spatially (i.e., specific geographical locations, stationary and mobile activities) (Teweldemedhin, Marwala, and Mueller 2004; Cliff et al. 2018; Hunter, Mac Namee, and Kelleher 2019).

Although this section considered just two applications of ABMs briefly, they outline credible ways in which heterogeneity can be represented, as its presence is critical to the design of successful interventions of any complex systems (Wallace and Ogawa 2015). From this brief discussion, two challenges when capturing heterogeneity have been identified: First, there is no standard definition for heterogeneity, nor is there a framework or guideline that constitutes the types or uses across disciplines. The second challenge lies in the discerning of an appropriate level of heterogeneity to include in models, that would adequately represent the given research objective (Smajgl, Bohensky, and Bohnet 2007). That being said, deriving an all-encompassing definition of heterogeneity that

applies to all possible ABMs across various disciplines and purposes is an impossible task; neither could an appropriate level of heterogeneity be specified, and it is important to recognise this.

However, what is clear is the following: specifying the appropriate degree of agent heterogeneity which satisfies specific research objectives remains a fundamental challenge. When the research objective or modelling goal is to explore macro-level consequences of theoretical preferences or behaviours, then the researcher may prefer to formulate behaviours that correspond to theory. However, if the goal of the model is to understand the micro-level consequences of real-world phenomena, then the formulation of agent behaviours must be empirically defensible (Hedström 2005; Bruch and Atwell 2015). Most real-world complex systems contain varying degrees of heterogeneity due to differences in the component properties. These differences can have radical impacts on the system's functioning and overall dynamics (Fisher and Pruitt 2020). When modelling systems which relate to humans, an animate object, it is important to consider that individuals are diverse in their biology (i.e., genetics, microbiome, blood types), behaviours (i.e., psychology, personality, decision-making propensities) and demographics (i.e., socioeconomic status, racial identities, age, sex). Thus accommodating such diversity creates a rich representation of the system and will result in successful interventions.

To facilitate the investigation into the impact of heterogeneity, the following section continues the review of the literature but differentiates between the *agent type*, as each type has unique attributes that structurally describe each agent. Two agent types are proposed: animate and inanimate agents. Agents are representations of autonomous entities within the boundary of a model, they can take on any form or structure (i.e., humans, buildings, cars, land parcels, water droplets or insects). Humans are animate, with an exclusive list of structural descriptors (i.e., age, gender, weight etc.) that would be different to structural descriptors of inanimate agents like organisations or agricultural products (i.e., size, density and location). It is important that these differences in structural descriptors are acknowledged, as they each have a significant impact on system dynamics. However, given the scope of this research, this section will only present the approaches in which heterogeneity has been displayed in animate agents.

2.5.1 Animate Agent Heterogeneity

As previously mentioned, an example of animate agents are humans and there are a plethora of ABMs which have studied population dynamics across multiple disciplines. For example, in studies which are used to simulate urban land-use change phenomena, such as residential segregation, agents are categorised by their preferences for co-ethnic contact. These types of models tend to be spatial, as the interactions agents have with each other are equally as important as the interactions they have with the environment.

Brown, Robinson, et al. (2008) modelled the complex processes of land-use and land-cover change in exurban parts of Southeastern Michigan. Their model described the evolution of the urban form as a consequence of residential preferences. In their agent-based model, there were four agent typologies or actors: residential land purchasers, developers, farmers and townships. All actors had their own specific behavioural rules which corresponded with their typology. A township represented an area, which was divided into farms. Farmers would then offer up parts of their farms for sale, which were ill-suited to their needs i.e., poor-quality soil land or areas located near county roads. Developers would determine how and what the area would be used for depending on lot size, effects on tree cover and proximity to amenities. Additionally, developers are driven by residential demand for particular lot types. Residential land owners or residents were characterised with variable preference weights for environmental characteristics and heuristics describing their desired lot type. Their preference weights and lot choices were determined by their socioeconomic characteristics, including income, parental status, and whether or not they belonged to an environmental group. These heterogeneous attributes and preferences were derived from survey responses and factor analysis (Fernandez et al. 2005). The residential agent's main objective was to maximise their utility, but their rationality was bounded by incomplete information about the real estate market. Following some analysis, Brown, Robinson, et al. (2008) found the simulations which included heterogeneous residential preferences exhibited more sprawling and fragmented patterns than the homogeneous runs; agents achieved higher levels of average utilities. They concluded that the distribution of residential preferences and behaviours affected settlement patterns; this indicates that the inclusion of different agent types and corresponding typologies

significantly impacted the overall dynamics of the model. In other words, agent heterogeneity is captured in both the categorisation of agent types e.g., having four agent typologies: residential land purchasers, developers, farmers and townships. Also, agent heterogeneity is captured in the variability in the agent attributes e.g., residents having different preference weights indicates a desired environment choice unique to the agent. By including comparative homogeneous and heterogeneous agent scenarios in the study, the impact of agent heterogeneity on residential preferences was made observable.

In addition, Wahyudi, Liu, and Corcoran (2019) investigated different land developers' behaviours and their consequences on urban development in Jakarta, Indonesia. In their agent-based model, developers were the only agent type but there were three typologies: small, medium and large developers, where their size denoted capital resources, and lending capacities and development preferences. The developer's characteristics were determined by interviews with experts in urban development, literature studies and newspaper articles. They compared the results of homogeneous simulation (i.e., scenarios where all agents were either small, medium or large), to heterogeneous simulations (i.e., an equal hierarchical mix of developer typologies); they found that each developer typology produced significantly diverse spatial patterns. It confirmed that urban areas developed by small developers tend to have a small disconnected shape with high edge density and low clumpiness index (McGarigal and Marks 1995; Deng et al. 2009). Whereas, large developers produced more connected urban patterns with low edge density and high clumpiness index. In the heterogeneous cases, the spatial patterns produced were more mixed and complicated. There were also noticeable differences in simulated land prices: when compared to Jakarta's initial land value map in 1994, the marginal land value increased more in the heterogeneous scenarios than in the homogeneous scenarios of single-type agents. Wahyudi, Liu, and Corcoran (2019) found that larger developers were capable of selecting land in the most profitable locations, whereas smaller developers chose smaller blocks of land to develop, this resulted in a fragmented distribution of new urban areas. Despite modelling just one agent type, the diversity in typologies accounted for differences amongst developers which had rarely been included in other residential segregation models. With that said, researchers agree that developers play a critical role in shaping new developments, there are seemingly few studies that have attempted to model developer's behaviours to understand their direct impact on urban growth (Coiacetto 2001). As did the previous study, agent heterogeneity captured in the categorisation of agents into typologies and the introduction of variability in typology attributes proved to significantly impact the model dynamics and the overall results.

Moreover, Bruch and Mare (2006) used social survey data from the Multi-City Study of Urban Inequality (MCSUI) to build an agent-based model to investigate racial attitudes and racial residential segregation in contemporary urban America. The survey data identified some consequential results: at the time it revealed the overall unwillingness white people possessed to live in neighbourhoods with substantial presence of black people. Therewithal, they discovered a pattern that white people shared in neighbourhood preferences: the number of white people monotonically declined with an increase in black people. They categorised agents by two typologies: agents were either white or black. The monotonic pattern in white people's preferences was assumed to mean homogeneity in neighbourhood preferences. Therefore, white agents shared similar preference thresholds and the same average level of tolerance. Bruch and Mare (2006) compared different preference functions (i.e., Schelling-Sakoda threshold, Continuous Linear and Non-Linear, Nonzero Probability and the Staircase function) using the same average level of tolerance and identified differences in neighbourhood formation patterns. In comparing preference functions, it allowed for an evaluation of the underlying assumptions which governed agent mobility choices. In the Schelling-Sakoda threshold and staircase function simulations, the assumption that agents were indifferent to neighbourhood preferences resulted in higher levels of segregation. While in simulations which used the continuous and nonzero probability functions, the assumption that agents were more sensitive to changes in the neighbourhood proportion of their group, led to lower segregation. In that same way, Bruch and Mare (2006) simulated segregation with heterogeneous neighbourhood preferences, but found that allowing for heterogeneity did not change the results. In fact, the segregation observed in heterogeneous agents was identical to those observed for homogeneous agents.

On the other hand, Xie and Zhou (2012) treated the monotonic pattern in white people's preferences as different levels of tolerance for black neighbours. They introduced heterogeneity by

formulating six agent typologies, all with different tolerances which were informed by the MCSUI dataset; and found it significantly impacted the model results when compared to the Bruch-Mare model. They found that in the long term segregation under the heterogeneous model was notably lower than the Bruch-Mare results. Xie and Zhou (2012) attributed the difference to there being a small subset of the white agent populations with higher tolerances of the other race, which lowered segregation long-term. These studies examined the same phenomena, using the same data and methods, yet they produced significantly different results. The differences observed relate to how heterogeneity was presented: in the Bruch-Mare model agent heterogeneity was demonstrated through the varying neighbourhood preferences, compared to the Xie-Zhou model which formally categorised agents by tolerances. These models illustrate a critical point to consider: how agent heterogeneity is presented can impact model results. Although, heterogeneity in varying neighbourhood preferences had no impact on segregation in the Bruch-Mare model, heterogeneity in tolerances from the Xie-Zhou model changed the observed dynamics of the phenomenon. These studies capture agent heterogeneity in the categorisation and variability of typologies and attributes, but they also demonstrate how the choice of variable used to present agent heterogeneity can impact model results e.g., Bruch and Mare (2006) interpreted the monotonic pattern in preferences as homogeneous neighbourhood preferences, whereas Xie and Zhou (2012) interpreted the pattern as different levels of tolerance. Ultimately the interpretation of the monotonic patterns produced different model results.

Filomena et al. (2022) simulated pedestrian movement in urban areas incorporating behavioural heterogeneity in pedestrian route choice strategies using agent-based models. They studied how variation in agent attributes could impact movement patterns using survey data collected in Münster, Germany. Agent heterogeneity was presented in agent attributes: they identified six clusters with differing likelihoods of engaging in walking trips for different purposes. When compared to the homogeneous population where all agents shared a similar likelihood of walking trips, Filomena et al. (2022) observed very few differences in pedestrian flows in the heterogeneous case with six agent typologies. They claimed that movement patterns which emerged from the heterogeneous simulations were more plausible than in the homogeneous simulations. However, in running their model multiple times there were no observable differences between the homogeneous and het-

erogeneous simulations on this global urban scale; a phenomenon observed in previous works on residential choice (Buchmann, Grossmann, and Schwarz 2016). Although the impact of heterogeneity in pedestrian route choice is seemingly insignificant here, there remains an effort to identify other key individual aspects for which its heterogeneity may alter the model dynamics. As in the Segregation studies, how agent heterogeneity is presented matters too. An example would be to investigate the impact peer influence would have on pedestrian route choice strategies, which is evident in studies examining emergency evacuations. Generally speaking, choices are rarely made in isolation, there are always contributing factors. It is well-established that exposure to others' decisions may influence an individual's own (Baddeley 2010), specifically on route choice in urban networks or built environments (Papadimitriou, Yannis, and Golias 2009; Kinateder et al. 2014). As mentioned above, the impact of heterogeneity is insignificant here, but this may depend on how it is presented. In addition to that, the impact of heterogeneity is observable in cases with agent interaction as they tend to lead to surprising deviations in the resulting patterns (Brown, Page, et al. 2005; Railsback 2019). It is possible that in adapting the model to accommodate the above, the impact may become observable in pedestrian movement models. This study demonstrates the capturing of agent heterogeneity in the categorisation and variability in typologies and attributes. In addition, it presents a supporting case for the use of comparative homogeneous and heterogeneous scenarios. Although the clustering identified from the survey data presented motivation to model agents heterogeneously, it was only in modelling both homogeneous and heterogeneous scenarios that an impact could be observed. This comparative study presents as an example whereby increased granularity or heterogeneity fails to further enrich the model's explanatory or predictive power.

Similarly, Muhammad et al. (2018) employed a microscopic approach to investigate crowd simulation using flocking behaviour characteristics (Reynolds 1999). The microscopic approach presented heterogeneity through variability in agent attributes, whereas the macroscopic approach would assume crowds were homogeneous to study aggregate effects. Their microscopic model categorised agents into two agent typologies: independent or cooperative agents. Independent agents were affected only if they observed another agent being influenced to respond differently to their environment. In this way, just the presence of an influential agent could affect decisionmaking but not result in cooperation. Cooperative agents were considered dependent, in that their behaviour would be directly impacted by inter-agent communication; they were either leaders or followers. For navigation, each agent used its own finite-state machine to seek out their destinations, but they were all equipped with different speed capabilities. In simulations where agents were homogeneous in speed and relations, there was the least number of collisions; and on average, these simulations had shorter running times. In comparison to the heterogeneous simulations with variance in agent's speed and relations, there were a higher number of collisions and longer running times. Muhammad et al. (2018) proposed the differences in simulation running times were due to agents taking longer to navigate from the start to the destination. Interestingly, they found that leader agents tended to have dense crowds of follower agents; the denser the crowds around a leader, the more collisions were experienced. Choosing to investigate flocking behaviour microscopically, allowed the researchers to examine the individual interactions which lead to a display of collective behaviour. Another fascinating viewpoint: outside of the heterogeneity initialised into the model through speed and relations, the heterogeneity observed evolved. This was indicated by the increased collision rates, which changed agents' speed and relations i.e., independent agents being influenced into exhibiting Cooperative "follower" behaviours. Further study into generative heterogeneity, especially in crowd simulations, is imperative. Agents within the heterogeneous scenario not only had varying speeds and relations, but they also had their finite-state machine leading to heterogeneous interactions with the environment and each other. As collective behaviours, such as crowds, result from individual interactive objects, monitoring heterogeneity that was generated may have uncovered further significant results. In this study, modelling agent heterogeneity in crowd simulations produced realistic simulations of high-density crowds.

Furthermore, Entwisle et al. (2016) examined the effect of climate shocks on migration in rural agricultural areas using a combination of empirical survey and ethnographic data from the Nang Rong District, Thailand. They categorised agents into five types: individuals, land parcels, house-holds, social networks, and villages. The model explored agent migration response to four different climate scenarios. They investigated the effect individual characteristics had on migration and found very few differences in migration rates in homogeneous and heterogeneous simulations. The individual characteristics considered were attributes such as age, gender, marital status and other

socio-demographic descriptors. Household agents had attributes such as assets, land ownership, centrality of the household in village networks, and ties to the wealthy. Land parcels had attributes, such as size, distance from the village, flooding potential, land use type, and soil suitability for various agricultural uses. Finally, villages had attributes that aggregate individual, household, and parcel attributes (e.g., population size, migration prevalence) as well as a social network variable (connectivity). This suggested that while heterogeneous agent characteristics were an important component of migration, they did not significantly impact migration response to extreme climate scenarios. Entwisle et al. (2016) reasoned that most rural agricultural areas had pre-existing conditions to migrate even when experiencing 'normal' weather; in this case, migration could not be established as a direct response to climate change. Further, they argued that the true impact of heterogeneity was dulled by the pre-existing condition of the environment. To identify the impact agent heterogeneity has on migration due to climate shocks, a comparative study of areas not typically characterized by high migration in response to extreme climate would need to be undertaken. Although the impact of agent heterogeneity is seemingly insignificant it does raise another important point: the presence of detected pre-conditions can affect the observability of the true impact of agent heterogeneity on system dynamics.

In less spatially explicit ABMs, specifically economic or financial models, heterogeneous interacting agents have been richly documented (Chiarella, Dieci, and He 2008; Hommes and Wagener 2009; Lux 2009; Westerhoff 2009). Standardly, economic models assume an individual's expectations are formed rationally (Muth 1961). To form rational expectations means on average individuals make rational decisions, informed by access to unlimited information and possession of perfect analytical skills. For some time, only representative agents informed by the rational expectation assumption were used to observe and study the dynamics of the macroeconomy (Nature 2009). By using representative agents, researchers could assume homogeneity to simplify the complexities of individual differences introduced to consumers' interactions with the real economy. However, Tesfatsion (2002) proposed agent-based models as an effective modelling technique for economic processes, called agent-based computational economics (ACE). In ACE, rather than modelling a single agent as a representative, the behaviour of whole populations through multiple agents could be observed. The individual economic interactions occurring on a micro-level could be linked to what was observed on the macro-level. This research area demonstrates the impact and significance of agent heterogeneity as researchers have been able to reproduce market dynamics observed in real financial markets.

Bertella et al. (2014) used an agent-based model to study the impact of behavioural bias in financial markets. They constructed an artificial stock market comprised of two agent typologies: fundamentalists and chartists to model different decision-making processes. Given their typology, each agent would utilise a specific strategy to evaluate stock prices; in addition to this, each agent would have different memory length and confidence levels. Fundamentalist agents would estimate the future value of the stock by using the future Discounted Dividend Flow Model (Gordon and Shapiro 1956; Gordon 1959), whereas Chartist agents keep track of past average prices to inform future decisions and they can either be trend followers or trend contrarians. To explore the dynamics of the artificial stock market, Bertella et al. (2014) carried out a series of simulations. In the homogeneous simulations, agents were all fundamentalists with the same decision-making strategy and they found the fundamental value of asset prices fully reflected all the information available to market agents. In the heterogeneous simulations with chartist agents that had varying memory lengths, they observed excess volatility and kurtosis, in agreement with real market fluctuations. In reproducing behaviours observable in real-world financial markets, Bertella et al. (2014) proposed differences in memory lengths as the main source of fluctuations in asset stock prices. Agent heterogeneity had a significant impact on model results, they demonstrated differences in how people process information and their confidence, which could directly influence real-world asset stock prices.

In further examples, specifically models which utilise information diffusion frameworks, agent heterogeneity has played an integral role in understanding how new ideas, technologies and practises can spread throughout a social system. This spread or diffusion acts as a movement flow between the source and an adopter, usually through some interpersonal communication or wider influence e.g., mass media (Rogers, Singhal, and Quinlan 2014). Most research on innovation diffusion has been based on the seminal work of Bass (1969). The Bass model contrives the aggregate level of penetration of a new product based on two communication processes: external influence

from advertising or mass media and internal influence from word-of-mouth. All consumers follow the same decision-making process described as a probability to adopt the new product during a time and depend linearly on internal and external influences. The Bass model and other variations have been utilised to explain different aspects of diffusion (Mahajan and Muller 1979; Mahajan, Muller, and Wind 2011), and they hold a significant amount of value. However, a shortcoming of Bass is the assumption that all consumers are homogeneous; it did not consider how a consumer's decision-making, communication and influence could evolve or change over time. One of the first examples of agent heterogeneity in innovation diffusion modelling was Chatterjee and Eliashberg (1990). Chatterjee and Eliashberg (1990) presented an analytical model based on individual decision-making that determined the adoption of agents one by one. The decision to adopt was dependent on a set of consumer characteristics e.g., perception of innovation, personal preferences and perceived reliability of the information they received. Building on this, Delre, Jager, and Janssen (2007) built an agent-based diffusion model which studied how social processes could affect diffusion dynamics and how the speed of the diffusion depended on the network structure and on consumer heterogeneity. Agent heterogeneity was introduced through the allocation of personal thresholds which determined whether they would choose to be involved or not in a group behaviour. Delre, Jager, and Janssen (2007) found when compared to homogeneous simulations where agents shared the same threshold, the heterogeneous simulations resulted in faster diffusion speeds. The Bass Model remains a popular method used to explore information diffusion, most especially when examining aggregate effects. However, in proposing that consumers as heterogeneous, the observable dynamics of information diffusion change. This suggests that the impact of agent heterogeneity may be dependent on the object of study, it could be that homogeneous assumptions most appropriately capture system dynamics.

Comparably, there is a significant amount of research exploring the impact of heterogeneity in network structures in innovation diffusion models. Classically, an aggregate diffusion model would assume that innovation adopters would have the same chance of communicating with everyone within the network; whereas newer models allow for heterogeneous interactions which assume innovation adopters may have a limited set of interactions within the social network (Midgley, Morrison, and Roberts 1992; Valente 1995). Bohlmann, Calantone, and Zhao (2010) studied the impact

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interpersonal communication between adopters could have on the diffusion process; their goal was to understand how adopter's network connections could affect innovation diffusion. The two types of heterogeneities they addressed were structural and relational. Where structural heterogeneity referred to the different social network structures that could arise amongst a select number of adopters but not all (Thieme 2007); and relational heterogeneity emerged from varying strengths and degrees of interpersonal communication amongst connected adopters (Goldenberg, Libai, and Muller 2002). Bohlmann, Calantone, and Zhao (2010) found network topology had a more pronounced effect on diffusion processes for higher adoption thresholds (i.e., the more difficult innovation is to diffuse). To investigate relational heterogeneity, the agent population was divided into two types: innovators and followers. In application, the nature of relational heterogeneity, specifically for marketing efforts, suggests taking advantage of the most influential communicators to avoid a short initial period of sales followed by a noticeable trough. To avoid these troughs they suggest targeting the innovators or 'opinion leaders' of the community first to ensure the follower agents adopt and eventually saturate the market. The impact of agent heterogeneity within the context of this product diffusion study was significant; this study proposed that only understanding the communication influences within a heterogeneous network structure, could inform decisions regarding effective marketing decisions be made. Moreover, if agent interactions generate network effects (Bonabeau 2002), then the types and effects of heterogeneity found in network sciences could be applied to this study of heterogeneity in agent-based models. Structural heterogeneity refers to the structural changes that would arise as a direct result of agent heterogeneity; relational heterogeneity would emerge directly from agent interactions. However, as individual behaviours in agent-based models are considered nonlinear, there may be difficulty in distinguishing between the effect of structural and relational heterogeneity.

In light of the above analysis, several critical points to consider when investigating the impact of agent heterogeneity have been formed. Firstly, comparative studies of homogeneous and heterogeneous scenarios should be considered a standard; only in doing so can the impact of heterogeneity be observed. Secondly, agent heterogeneity is often presented in two forms, which should be considered non-mutually exclusive: categorisation and/or variability of the agent population and attributes. Studies which used categorisation (typologies) would categorise agents by a specific

agent attribute; to do this there would have to be an indication of an underlying assumption that agent characteristics or attributes were correlated. Studies which used variability would also distinguish agents by typology and in addition, would vary agent attributes and characteristics values, informed by real or simulated data. Thirdly, agent heterogeneity is introduced in the model initialisation stage but rarely is the evolution of the initial heterogeneity ever monitored. The type of heterogeneity which was developed from initial conditions can be referred to as generated heterogeneity. Fourthly, the choice of the variable used to demonstrate agent heterogeneity should be considered when evaluating the impact of heterogeneity on results. Fifthly, there may be some undetected preconditions between agent attributes and characteristics that could affect the observable impact of agent heterogeneity on model results. If agent heterogeneity is seemingly insignificant, researchers should consider the potential existence of underlying relationships that could obscure the observability of significance.

The sixth and final point, the target system (i.e., the object of study or the system being modelled) and research purpose are factors to consider when choosing between homogeneous or heterogeneous assumptions, it is possible that the target system may have a predisposition to one more so than the other. Though these points are critical, they only cover studies with animate agent objects. In addition, this review includes spatially explicit ABM literature but it does not consider the impact differences in the spatial location of an agent (and the location's attributes) have on the model results. Including heterogeneity in location attributes veers the study from the agent component to the environment component¹. As the objective of this thesis is to establish the impact of agent heterogeneity exclusively, the emphasis is on agent components and not the environment components of ABMs.

2.6 Summary - Agent-Based Models

This chapter presented agent-based models as a method for modelling complex systems. The popularity of agent-based models has been attributed to their flexibility in application; this chapter proposed heterogeneity as its source. Within the scope of this research, heterogeneity was defined

¹ABM components were outlined in Section 2.4.1.

as agent granularity, which would refer to the *coarseness* of descriptive attributes and behaviours assigned in the agent component (Gao, Song, and Wang 2013).

Having established the agent-based model framework, the role and potential impact heterogeneity may have on system dynamics, the following chapter will briefly review the literature relating to modelling emotional contagion as an agent-based model.

Chapter 3

Understanding Emotional Contagion

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3.1 Chapter Overview

The objective of this research is the study the impact of heterogeneity in agent-based models using emotional contagion as a case study. To develop this model, a comprehensive understanding of the dynamics of contagion is imperative. This chapter will explore models of emotional contagion as collective behaviour, with a focus on infectious disease frameworks. To begin, Section 3.2 will outline forms of collective behaviour. Section 3.3 will explore the proposed theories of collective behaviour with a focus on contagion theory. Lastly, Section 3.4 will outline compartmental models as an approach to modelling emotional contagion.

3.2 Collective Behaviour

A recent example of collective behaviour occurred during the early stages of the global pandemic in 2020. As a result of this period of uncertainty, individuals experienced extreme cases of fear, panic and anxiety (Lins and Aquino 2020). In response to the media coverage of global shortages of toilet paper, hand sanitiser and food supplies, there was a sharp increase in the purchase of these items (Bentall et al. 2021). Panic buying is defined as a behavioural phenomenon that occurs in response to environmental stressors (Cooper and Gordon 2021). In essence, it is a display of *collective behaviour*, an instance where the behaviours of heterogeneous or homogeneous populations governed by their social norms are abandoned, and the population combine to present a singular common display of behaviour.

An objective of collective behaviour research is to both understand and predict how collective patterns emerge from the behaviour and social interactions of individuals (Jolles, King, and Killen 2020). Collective behaviour research is an interdisciplinary field which has utilised quantitative approaches of physicists, computer scientists and mathematicians to investigate underlying mechanisms (Ioannou and Laskowski 2023). Through the theoretical and experimental work of social scientists, they agree that many complex collective behavioural patterns can emerge through self-organising processes using simple interaction rules (Bonabeau et al. 1997; Parrish, Viscido, and Grünbaum 2002; Sumpter 2006; Herbert-Read 2016). Collective behaviour has been studied in animal populations (Sumpter 2010; Aplin et al. 2014; Ward and Webster 2016; Hughey et al. 2018) and humans (Dyer et al. 2009; Goldstone and Gureckis 2009; Smelser 2013; Whiten et al. 2022) using agent-based models (Macy and Willer 2002; Kleinmeier, Köster, and Drury 2020). Thus, this study of collective behaviour, specifically the modelling of emotional contagion, serves as an adequate example that enables the display of homogeneous and heterogeneous population tendencies.

3.2.1 Forms

This section will briefly present different forms of collective behaviour and the extent proximity is a useful criterion in the digital age. The most common forms of collective behaviour can be differentiated by whether or not the actors need to be in close proximity. Crowds, panics, riots and disaster behaviour involve physical interaction between the participants (Tilly 1992). In contrast, rumours, mass hysteria, moral panics, and fads and crazes, are not constrained by geographical locations or physical proximity, the only requirement for participants is a shared belief or concern. This section will only explore a few examples of the forms and events of collective behaviour, therefore this review should not be considered exhaustive.

The most obvious form of collective behaviour, particularly where physical proximity and geographical location are present is a crowd. Crowds are the only form of collective behaviour acknowledged and included by all scholars and authors. Blumer (1995) identified four types of crowds (i.e., large groups of people): the casual crowd, the conventional crowd, the expressive crowd and the acting crowd. When defining these crowds, Blumer considered the varying degrees of emotional intensity they may exhibit.

Casual crowds are groups of people with little in common, and no shared purpose or identity. Participants of the casual crowd scarcely interact; an example is people gathered at a pedestrian crossing along a busy road. In this case, a temporary common goal between participants to cross the road exists, but quickly dissipates once the goal has been reached. Goode (1992, p.22) emphasised that participants of causal crowds have nothing in common besides their physical location and, therefore may not truly be displaying collective behaviour as participants still follow conventional behavioural norms.

Conventional crowds are groups of people gathered for a specific purpose or planned event. Some examples include participants attending a movie, play, concert or lecture. As with casual crowds, Goode (1992) found participant behaviours to be relatively structured and would conform to the appropriate set of norms for the situation.

Expressive crowds gather to be excited and to express one or more emotions. These types of crowds include religious gatherings, political rallies and festivals such as Mardi Gras. The difference between conventional and expressive crowd activity lies in how participants view the assembly. In conventional crowds, participants being members of the crowd is secondary or irrelevant; their primary objective would be the consumption of the specific purpose or planned event.

Whereas in expressive crowds, participants desire to be members of these crowds and therefore participate in associated behaviours, by cheering, stomping, shouting and clapping (Goode 1992, p.23). It's important to note that the features of conventional and expressive crowds are not always definite. Conventional crowds may become expressive when displaying any emotional expression, as long as the crowd engages collectively. This suggests that crowds and crowd activity are not fixed behaviours and should be considered fluid.

The fourth and final crowd identified by Blumer was an acting crowd. Acting crowds would gather energetically to 'act on' a specific goal, they could be characterised as violent and destructive types of crowds as participants usually act on the basis of 'aroused impulse'. An example is a "mob" (Couch 1968). Mobs are an unruly and volatile emotional crowd that commit to pure violence, a recent example is the Pro-Donald Trump mob that stormed the US Capitol in 2021. Also, the killing of Mark Duggan by UK police in 2011 set off a wave of violence across the country. In addition to mobs, panic is an example of an acting crowd. This type of crowd acts on a sudden reaction that is often self-destructive. Section 3.3 will explore panic or emotional contagion in detail, but examples of panicked crowds include incidents where participants sustain life-threatening injuries during stampedes or evacuations. Acting crowds can grow exponentially in size and quickly out of control, to the extent of full-scale riots. Given the ideas discussed above, acting crowds are in effect the more violent extension of expressive crowds.

Although Blumer's work is widely accepted and considered the foundation of crowd behaviour studies, some alternative forms have been proposed. For example, McPhail and Wohlstein (1983) distinguished a fifth type of crowd, the protest crowd from the expressive crowd. As implied by its name, a protest crowd is a group of people gathering together to protest political, social, cultural, or economic issues. Some examples include demonstrations, marches, rallies and sit-ins. Further, Lofland (1991) proposed crowds as the origin of specific shared human emotions. Lofland identified three types based on three fundamental human emotions: fear, joy and anger. From fear, a panicked crowd could form; from joy, a crazed crowd; from anger, a hostile crowd.

A further form of collective behaviour contingent on geographical and physical proximity is disaster behaviour. When disasters occur, for instance, hurricanes, earthquakes, fires and floods,

standard routines are disrupted and survival is prioritised. During and after disaster impact, participants have to manage fears and anxieties whilst looking after their own and others' safety (Miller 2014, p.250). An intuitive belief regarding disaster behaviour is a display of selfish, individualistic and exploitative behaviour. However, current knowledge of disaster behaviour indicates that participant's reactions are more complex and context-dependent. Participants present diverse behaviours during a disaster depending on the severity of a hazard; meaning they tend to exhibit a wide range of unexpected reactions due to panic and stressful situations (Bakhshian and Martinez-Pastor 2023). Disaster behaviours can also change over time, whereby initial solidarity and altruism previously proposed by Goode (1992, p.181) can descend into social disintegration and decline (Ntontis et al. 2020).

To point out, the forms of collective behaviour outlined so far involve interacting participants within physical proximity discussed. As proposed earlier, however, some forms of collective behaviour are not constrained by the need for interaction or shared geographical locations. In spite of that, sociologists agree that these participants display collective behaviour through their shared beliefs and perceptions. Collective behaviours that involve shared beliefs and perceptions can be categorised into the following two groups: *1*) rumours, mass hysteria, and moral panics; and *2*) fashion, fads and crazes.

Rumours are uncorroborated and unverified assertions unaccompanied by evidence (DiFonzo, Bordia, and Rosnow 1994). Rumours can be presented in different forms including exaggerations, explanations, total fabrications and fears (Prasad 1935; Knapp 1944). Buckner (1965) regarded rumours as collective behaviour which through time, can increase or decrease in accuracy when being passed on; this variability is introduced through participant's individual interpretations.

Similarly, fashion and fads are impulses that are enthusiastically followed by large groups for a short period; they are seen as sudden, quick-spreading, and even referred to as crazes (Aguirre, Quarantelli, and Mendoza 1988). Fashion is an expressive form of collective behaviour, which does not aim to bring profound change to the social order, but rather should be viewed as "positive wish-fulfilment" (Smelser and Marx 1962; Horowitz 1975). Van Ginneken (2003) identified some differences between fashion and fads; the first being their distribution curves and the length of

time taken to fully saturate target groups. Classical fashion would have a very flat profile, indicating very little and slow changes to preferences. Normal fashion would mirror a bell-shape curve suggesting the annual pattern of preferences coming and going guided by the fashion industry and seasonal presentations. In contrast, fads have steep curves, indicating rapid adoption.

To summarise this section, collective behaviour can be categorised in terms of the physical proximity of the participants. However, it is important to emphasise that collective behaviour always emerges from interactions whether through close physical proximity or other forms of interactions. The following sections explore theories of contagion that underpin collective panic behaviour. There are many important types of collective behaviour, but the focus of the following sections will be on human behaviours.

3.3 Social Contagion as Collective Behaviour

This section will explore theories of collective behaviour; before focusing on explanations that describe collective behaviour as contagion.

3.3.1 Collective Behaviour Theories

Sociologists, psychologists and an assemblage of scholars have proposed many theories and explanations of collective behaviour over the years. These theories focus on explaining collective behaviours that involve little social interaction between participants, for instance, crowds, riots and social movements.

The main theories developed to explain these types of collective behaviours include:

- 1. *Convergence theory*: proposes participants of crowd behaviour hold and share similar beliefs and intentions, before joining a crowd (Allport 1924; Miller et al. 1941).
- 2. *Emergent norm theory*: proposes initially, participants are unsure of how to behave when beginning to interact in collective behaviour. They choose to discuss their potential behaviours and from this, societal norms emerge and a social order is created that governs subsequent displays of behaviour (Turner and Killian 1957).

- 3. *Value-added theory*: proposes collective behaviour as the result of preconditions; including generalised beliefs, structural strain and lack of social control (Smelser and Marx 1962).
- 4. Threshold model: proposes the existence of threshold effects in complex contagion, whereby participants observe the behaviour of others before deciding to join in. In essence, the stronger a participant's interest in the outcome, the lower the number of others needed to trigger that member's participation (Granovetter 1978).

Allport (1924) developed convergence theory which suggests crowd behaviour is a reflection of individual behaviour and attitudes of participants that join the crowd. Thus, crowds do not influence individual participants to act, rather their behaviour is a result of shared attitudes and beliefs. Convergence theory proposes crowds do not affect individuals instead individuals affect crowds. In essence, participants converge to a single mood, emotion, idea or issue and elicit herd behaviour in which they are connected to and process stimuli in a similar manner (Goode 1992; Raafat, Chater, and Frith 2009). Interestingly, in convergence theory crowds may act in a manner that individual participants are unlikely to; for example, when large mobs commit targeted violent acts. It can be assumed that the targeted attack by the mob is a result of individual personal beliefs or ideas of participants.

In contrast, Turner and Killian (1957) proposed emergent norm theory as an alternative explanation for collective behaviour. According to them, in the initial stages of collective behaviour participants are not entirely sure how to behave. As participants begin to interact, they discuss potential behaviour and settle on a select few governing norms; from this, 'new' behaviour emerges and this new social order and rationality continually guide group behaviours. Emergent norm theory views collective behaviour as less predictable than convergence theory, as before joining the crowd participants may not share similar beliefs or attitudes. Rather than participants converging to a specific cause, idea or issue, as indicated in convergence theory, emergent norm suggests participants allow for rationality and social order to guide behaviours.

The most popular explanation of collective behaviour and social movements is proposed by Smelser and Marx (1962). The value-added theory, often referred to as structural-strain theory, suggests preconditions must be present before collective behaviour or social movements can oc-

3.3. SOCIAL CONTAGION AS COLLECTIVE BEHAVIOUR

cur. Of these preconditions is the existence of structural strains, which refers to societal problems that anger or frustrate people. Structural strain serves as motivation for protests and the rise of similar social movements. Generalised beliefs are a further precondition for collective behaviour, these beliefs serve as reasoning behind poor conditions of societies and their proposed solutions for improvement. If people conclude their conditions are poor as a direct result of their decisions, they will not protest. In addition to this, if people deduce that protests and social movements will not improve conditions, they will not participate in protests. Further, a set of precipitating factors (sudden events) must exist that trigger collective behaviour. As mentioned in Section 3.2.1, a real example of an acting crowd in the UK was the series of violent protests which erupted across London following the killing of Mark Duggan by police in 2011 (Akram 2014). These violent waves were ignited by the contradictory and defaming news reports which falsely described the incident to the public. The final precondition is lack of social control which proposes collective behaviour as more likely if participants do not expect to be held accountable i.e., no threat of arrest or punishment, or being harmed. The value-added theory gained popularity by identifying several contributing factors that must hold true to facilitate a condition for the occurrence of collective behaviour or social movement. However, even if the preconditions are wholly satisfied, collective behaviour still may not occur. There is also a lack of clarity regarding the predictions; for instance, how much of these preconditions are necessary to initiate a display of collective behaviour (Rule 1988; White 1989). In comparison to both convergence and emergent theory, value-added theory removes focus from individual participants and broadens it to consider societal structures. The value-added theory proposes some underlying determinants that facilitate an environment for collective behaviour to occur.

Granovetter (1978) aimed to explain the emergence of collective behaviours in a manner which considered individual norms and preferences as crucial contributing factors to the outcome (Granovetter and Soong 1983, 1986, 1988). Under the threshold model, participants are presented with a simple binary choice to partake in a collective behaviour or not. To inform their decision, participants would have an reach a 'threshold' for participation. The threshold indicates the proportion of the wider group that chooses to partake in the display of the collective behaviour before a given participant chooses to join. An early example of thresholds was illustrated by Berk (1974) using

riots suggesting, that the cost of joining a riot declines as the number of participants increases, as the probability of being apprehended decreases. More recently, Grabisch and Li (2020) studied a threshold model where both conformist and anti-conformist participants coexist, rather than following the basic assumption that participants tend to follow the trend (they are conformist) and that nobody will have a kind of opposite behaviour (anti-conformism), choosing action 0 if too many people take action 1. Essentially thresholds emerge from the norms, preferences, goals and beliefs of each participant. The applications of this model or variations are not limited to simple crowd-like behaviours, but more broadly e.g., voting (Kaempfer and Lowenberg 1993), diffusion of innovations (Zeppini, Frenken, and Kupers 2014), migration (Hunter 2005), social movements (Lohmann 1994) and social tipping (Wiedermann et al. 2020).

An interesting consideration here is that none of the above theories fully explain all forms of collective behaviour; they simply propose alternative perspectives to explain the dynamics of collective behaviour.

3.3.2 Social Contagion

Plato's theory of mimesis was one of the earliest works that referenced the combined concepts of infection and imitation to explain human nature (Plato 1997). The figurative use of these concepts continued into early modern literature; contagion became a popular descriptive device for social phenomena through the work of Baldwin (1894), LeBon (1896) and Tarde (1903), on imitation and collective behaviour in 19th century France.

One of the earliest explanations of collective behaviour is contagion theory, which was first proposed by LeBon (1896) and has subsequently been examined in a wide range of work beyond sociology (Castellano, Fortunato, and Loreto 2009). LeBon's concerns were centred around the collapse of social order occurring during the French Revolution in the 18th century. At that time, mob violence was common in cities across Europe and the United States. The intellectuals and aristocrats viewed the violence as disturbing and a display of irrational behaviour; they saw participants as being under the influence of strong emotions and the opinions of charismatic leaders. These ideas served as the foundation of contagion theory. Contagion theory suggests individual

participants are rational until they form a crowd at which point they fall under hypnotic influence and act blindly out of emotion and irrationality. Participants under this influence lose control of their unconscious instincts and evolve into violence. This display of collective behaviour was likened to the dynamics of contagion, which passed the irrationality from person to person. In contrast, convergence, emergent-norm and value-added theories argue that strong emotions may influence collective behaviour, but those emotions are not irrational. In fact, Turner and Killian (1957) argue against the existence of contagion, as participants in collective behaviour do not lose the capacity to think and act rationally.

The term "social contagion" was coined by Herbert Blumer in his study of collective behaviour (Blumer 1939). Although empirical studies investigating social contagion have become more frequent; in those early days findings ranged widely as there was no shared definition. As a result, social contagion research has been described as incoherent and unorganised, lacking principles and conceptual framework (Levy and Nail 1993). For example, the Penguin Dictionary of Psychology defined social contagion as the spread or transmission of an activity or a mood through a population (Reber 1995). The Concise Oxford Dictionary of Sociology described social contagion as the flow or movement of ideas through a population (Marshall 1996). The Macmillian Dictionary of Psychology defined social contagion as the spread or transmission of ideas and feelings through a population by suggestion, gossip or imitation (Sutherland 1995). Other definitions have focused on the non-intentionality in transmissions, they suggest social contagion as the spread of an attitude or behaviour from an initiator to a recipient, where the initiator's actions, influential or not, are not perceived to be intentional by the recipient (Levy and Nail 1993). Contrastingly, some definitions explain social contagion as a type of inheritance, which are uncritical behaviours based on intuitive judgements rather than rational thinking; the Encyclopedic Dictionary of Psychology defined social contagion as the quick spread of emotions and behavioural patterns that are adopted uncritically within populations (Furnham 1988). There are some definitions that refer to disinhibition more so than the intentionality of transmission or inheritance. Wheeler (1966, p.180) define social contagion as:

If the set of test conditions T1 exists, then contagion has occurred if and only if Person

X (the observer) performs behaviour N (BN) where T1 is specified as follows:

- (a) A set of operations has been performed on Person X which is known to produce instigation toward BN in members of the class to which X belongs;
- (b) BN exists in the response repertoire of X, and there are no physical restraints or barriers to prevent the performance of BN;
- (c) X is not performing BN;
- (d) X observes the performance of BN by Person Y (the model).

With no standardised definition of social contagion, the studies produced have little in common except the observable phenomenon of spreading through contact. The definitions suggest the presence of individual internal states and mechanisms, such as intentionality and conflict, to explain the spreading process. Although important, understanding each individual component has overridden the fundamental need to understand the nature of social contagion. And the distinguishing of each individual component has made the study of social contagion more complex. These developments have deterred focus from the central rationale of the metaphor; which is, that the observable phenomenon spreads as if it has contagious properties (Marsden 1998).

The Handbook of Social Psychology has the clearest definition of social contagion since it refrains from placing caveats or further conditions on the process. It describes social contagion as the spread of behaviour amongst participants of a crowd and describes a single person as the catalyst for the transmission (Lindzey and Aronson 1985). This type of definition serves as an umbrella that more appropriately captures the scope of the phenomena. Unlike the other definitions, there is little focus on satisfying preconditions. Further, this broad definition can be applied to an array of social contagion examples, whether they be physical crowds or virtual social media/mass media crowds.

Additionally, there are thought to be two branches within social contagion: *behavioural* and *emotional* contagion. Behavioural contagion follows the spread of behaviour through groups. It focuses on the propensity of participants to mimic certain behaviours they are exposed to. The term 'behavioural contagion' was conceived to explain the disagreeable elements of crowd behaviours

3.3. SOCIAL CONTAGION AS COLLECTIVE BEHAVIOUR

(Stephenson and Fielding 1971). Digitally, behavioural contagion is concerned with the spread of online behaviour and information (Harrigan, Achananuparp, and Lim 2012). In addition to the above, an array of behavioural contagion mechanisms are incorporated in models of collective human behaviour (Castellano, Fortunato, and Loreto 2009). A prominent theory of behavioural contagion was proposed by Redl (1949) and further analysed by Wheeler (1966), which proposed the phenomenon as the result of the reduction of personal restraint (i.e., self-control). Some social psychologists suggest a number of factors that influence the likelihood of behavioural contagion for instance, deindividuation and the emergence of social norms (Festinger, Pepitone, and Newcomb 1952; Turner 1964). Likewise, Freedman, Birsky, and Cavoukian (1980) focused on the effects of physical factors on behavioural contagion, specifically density and number. Ogunlade (1979) described behavioural contagion as "spontaneous, unsolicited and uncritical imitation of another's behaviour" which occurs following the satisfaction of preconditions. For example, the initiator and recipient share a similar situation or mood and the initiator's behaviour would encourage the recipients to review their condition and motivate a change.

On the other hand, emotional contagion involves the spontaneous transmission of emotions overtly or covertly through groups. A broader definition proposed emotional contagion as an example where the initiator influences the recipient consciously or unconsciously to adopt certain emotional states or attitudes (Schoenewolf 1990). It has been proposed that emotions may be transmitted through facial expressions, voice, posture, movements, and other instrumental behaviours (Hatfield, Cacioppo, and Rapson 1993). Facial expressions were considered a form of nonverbal communication used to display a range of emotions (Brown 2004). Some laboratory studies have proven the existence of emotional contagion, where the recipient participant displayed an emotional response that mimicked the emotions expressed by the initiator participant (Lundqvist 1995; Hess and Blairy 2001). Researchers attribute mimicry to an attempt for people to empathise with each other (Barger and Grandey 2006).

Be that as it may, following on from Granovetter (1978), collective behaviours such as social contagion have been understood to spread through social contact. But when these behaviours are controversial, participation requires independent affirmation or reinforcement from multiple

sources (Centola and Macy 2007). Therefore, social contagion has been further defined as a type of *complex contagion* whereby successful transmission depends on interaction with multiple carriers. Social contagion is considered complex for several reasons, such as the need for social legitimisation, the need for credibility, or the complementarity of a behaviour, externalities and uncertainty (Guilbeault, Becker, and Centola 2017).

For example, public health studies have been linked to both biological and social contagions. It is suggested that simple contagions do not adequately capture the network dynamics that govern the diffusion of health behaviours as they require reinforcement from peers and are strongly influenced by cultural practices and group norms (Centola 2010, 2011). Christakis and Fowler (2007) conducted the Framingham Heart Study and found obesity spread socially through a densely interconnected network of 12,067 people, assessed between 1971 to 2003. They found that either biological or normative mechanisms are expected to yield very different diffusion dynamics. Similarly, a series of studies have demonstrated how clustered networks that facilitate the spread of social norms, such as anti-vaccination behaviours, can make populations susceptible to epidemic outbreaks of simple contagions, such as measles (Salathé and Bonhoeffer 2008; Campbell and Salathé 2013; Fügenschuh and Fu 2023). These studies examine the diffusion of anti-vaccine attitudes as echo chambers which intensify the likelihood of disease outbreaks through the wider population; echo chambers are an example of complex contagion (Törnberg 2018).

Furthermore, the diffusion of technological innovations through populations is seen as a complex contagion, rather than simple as first proposed by Bass (1969). For instance, Bandiera and Rasul (2006) found that the adoption of new crops by farmers in Mozambique would depend on their number of network neighbours who had already adopted it. Oster and Thornton (2012) illustrated the adoption of women's menstrual cups depends on influence from multiple peers who transferred technology-relevant knowledge. Billard (2021) found that under a complex contagion approach, the diffusion of green technologies may be affected by the social network structure, social dimensions and the technologies' learning effects. The complex contagion approach has been examined empirically across a variety of domains, including social media (Kooti et al. 2012; Mønsted et al. 2017) and politics (Romero, Meeder, and Kleinberg 2011; Traag 2016; León-Medina

2023).

Recent work aimed at investigating the transmission of social contagion throughout groups and whole populations has involved researchers across a range of disciplines, from psychology, and sociology to network science. Although social contagion was originally theorised, defined and modelled using a simple contagion approach e.g., a single source can be sufficient for transmission, now social contagion is more widely accepted as a type of complex contagion e.g., transmission relies on contact with multiple sources of infection. Having now understood the complexity behind social contagion mechanisms and dynamics, to sufficiently investigate the impact of heterogeneity in agent-based models a simple case study model is required. Therefore, this study will consider emotional contagion within the context of a simple contagion. The following section will explore compartmental models in epidemiology as a methodology to investigate emotional contagion.

3.4 Modelling Emotional Contagion

Human behaviour and emotions are inherently complex, meaning they do not develop smoothly or logically (Brown 1995). Notwithstanding, mostly analytical models have been used to study social behaviours sciences (Rodgers, Rowe, and Buster 1998). Analytical models are well accepted amongst researchers and policymakers, as they are mathematically tractable and simple to fit empirical data. That being said, the more complex the social-behavioural model, the more challenging it is to solve analytically. This study will model emotional contagion using an ABM in Chapter 4, but to develop a model it must be informed by a framework. To identify which framework to use, the following subsections will briefly outline compartmental models as an approach to modelling contagion. This study uses the mathematical tool developed by epidemiologists to study the spread of emotional contagion, as these compartmental models can be generically used to study the dynamics of social, cultural and political change.

3.4.1 Compartmental Models

Compartmental models are a popular tool used to study the mechanisms by which diseases spread and to predict and mitigate future courses of outbreaks (Daley and Gani 2005). Compartmental models are generally expressed mathematically; the underlying statistical assumptions simplify the parameterisation of the infectious disease model to calculate the effects of different interventions. The first mathematical model used to study infectious disease dates back to a seminal paper published by Daniel Bernoulli in 1766 in support of smallpox inoculation. Bernoulli's calculations helped to illustrate how widespread inoculation would increase life expectancy by three years (Bernoulli and Blower 2004). By the 1920s, the development of compartmental models produced two more formative works: Kermack and McKendrick (1927) and Reed-Frost Epidemic Process (1928). These models were able to describe the relationship between susceptible, infected and immune groups within a population. Furthermore, Kermack and McKendrick (1927) successfully predicted behavioural patterns of outbreaks, which mirrored patterns that were observed from previous epidemics (Brauer and Castillo-Chavez 2012).

Susceptible-Infectious-Recovered (SIR)

After years of development, compartmental models are considered the primary method for modelling infectious diseases. The simplest example of a compartmental model is the Susceptible-Infectious-Recovered (SIR), which consists of the following three compartments (Harko, Lobo, and Mak 2014; Kröger and Schlickeiser 2020):

- Susceptible, S: represents the proportion of susceptible individuals within the populations.
- Infectious, *I*: represents the proportion of infectious individuals.
- Recovered, *R*: represents the proportion of previously infectious individuals that recover or have died. This compartment may also be referred to as removed or resistant.

The dynamics of the classical SIR model are visualised in a diagram, see Figure 3.1.

The SIR model is a fairly strong predictive tool for human-borne infectious diseases where recovery provides a degree of immunity (Yang, Zhang, et al. 2020). The variables S, I and R depict the proportion of individuals in each compartment at a certain time; this proportion may fluctuate in time even if the total population size stays constant. To accommodate for this the susceptible, infectious and recovered proportions are expressed as functions of time, t: S(t), I(t)



Figure 3.1: Diagram of Susceptible, Infectious and Recovered Model and Compartmental Transition Rates

and R(t). A strength of this model is its applicability, it can be widely applied to investigate and predict outbreaks and control measures for diseases across populations.

The SIR model can be adapted to accommodate for the inclusion or exclusion of vital dynamics i.e., births and deaths. The dynamics of some infectious diseases, such as the common cold or influenza, are expeditious when compared to the dynamic of birth and death, thus these tend to be excluded from such models. In omitting vital dynamics, the SIR model can be expressed by a set of ordinary differential equations:

$$\frac{dS}{dt} = -\frac{\beta SI}{N},\tag{3.1}$$

$$\frac{dI}{dt} = \frac{\beta SI}{N} - \gamma I, \text{and}$$
(3.2)

$$\frac{dR}{dt} = \gamma I. \tag{3.3}$$

Although this model is non-linear it can be solved analytically (Harko, Lobo, and Mak 2014). Furthermore, the dynamics of the infectious compartment depend on the basic reproduction ratio

$$R_0 = \frac{\beta}{\gamma},$$

which suggests that the basic reproduction ratio R_0 of an infection is the expected number of further infections spread by one infectious individual, where all individuals are susceptible and have no immunity (Fraser et al. 2009). R_0 is derived from the ordinary differential equations used to describe the SIR system and is affected by the duration of infection, disease infectiousness and the number of infectious individuals that have been in contact with the susceptible (Delamater et al. 2019). Generally, the larger R_0 the more infections, which become hard to control; the smaller R_0 the less likely the infection is to spread.

When choosing to include vital dynamics, the SIR model can be expressed as the following:

$$\frac{dS}{dt} = \Lambda - \mu S - \frac{\beta SI}{N},\tag{3.4}$$

$$\frac{dI}{dt} = \frac{\beta SI}{N} - \gamma I - \mu I, \qquad (3.5)$$

$$\frac{dR}{dt} = \gamma I - \mu R, \tag{3.6}$$

where Λ denotes the birth rate and μ is the death rate of the population. In this case, the basic reproduction ratio, R_0 is:

$$R_0 = \frac{\beta}{\mu + \gamma} \tag{3.7}$$

(Beckley et al. 2013). To model infections that do not have long-lasting immunity, such as the common cold or flu, a more appropriate model is the Susceptible-Infectious-Susceptible (SIS) model. Alternatively, there are versions that model periods of latency where individuals may not be infectious, these are the Susceptible-Exposed Infectious-Susceptible (SEIS) and Susceptible-Exposed Infectious-Recovered (SEIR) model variations.

Susceptible-Infectious-Susceptible (SIS)

In this thesis, a version of the Susceptible-Infectious-Susceptible (SIS) model will be used in Chapter 4 to investigate the impact of heterogeneity in ABMs. Figure 3.2 summarises the SIS framework.

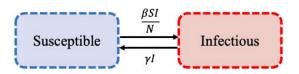


Figure 3.2: Diagram of Susceptible, Infectious and Susceptible Model and Compartmental Transition Rates

Unlike the SIR model, the SIS model has only two compartments: the Susceptible and Infectious. These models are most useful for modelling epidemics that do not have long-lasting immunity, such as the common cold or the flu. But as with the SIR model, the SIS transition rates are the same, as shown in Figure 3.2. Where $\frac{\beta SI}{N}$ can be summarised as the proportion of newly infectious individuals who were previously susceptible. And γI is the recovery rate of the individuals in the infectious compartment. Similar to SIR with no immunity, in SIS a constant rate of recovery exists which implies the number of recovered infections would be proportional to the size of the infectious compartment (Kuhl 2021).

Susceptible-Infectious-Susceptible-Spontaneous (SISa)

In more recent times, variations of the SIR and SIS models have been used to explain the spread of emotions and sentiments. Notably, Hill et al. (2010) modified the SIS model to not only demonstrate the spread of emotions through contact but also to account for the spontaneous transmission of emotions. To capture this they supplemented the standard SIS model with an additional parameter, *a*, to capture the spontaneity of emotional infection at a constant rate, independent of their infectious contacts. This version of the classical SIS model was named the Susceptible-Infectious-Susceptible-Spontaneous (SISa) model. Figure 3.3 illustrates the modified compartments and transition rates.

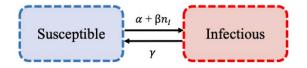


Figure 3.3: Diagram of Susceptible, Infectious, Susceptible and Spontaneous Model and Compartmental Transition Rates

The transition rate between the susceptible and infectious compartment is $\alpha + \beta n_I$, where *a* is the rate where a susceptible individual *automatically* becomes infectious, β is the rate at which an infectious individual transmits the infection to a susceptible individual and n_I denotes the number of infectious contacts.

In this novel approach, Hill et al. (2010) developed SISa to investigate emotions on a social net-

work. They defined emotion as a scale containing three levels increasing in duration and permanence, that would be subjective to each individual: fleeting moods, transitory states or personality traits. They defined their focus as the examination of transitory states, which they referred to as "long-term emotional states". They limited the types of long-term emotional states to just two, individuals could either be 'content' or 'discontent'; these terms had been likened to happiness and depression in previous works. Having established a framework and model, Hill built a social network using survey data from the Framingham Heart Study (Dawber 1980) to validate whether the data fit the dynamics of an infectious disease. Following some parameter estimation and further analysis, they proved that long-term emotional states could be spread between individuals who were connected socially. Their findings provided evidence in support of emotions exhibiting a transmissive nature. They summarised that the 'catching' of content and discontent emotions depended on social contacts, whereas recovery to a neutral state did not. However, they concluded that the mechanisms behind the transmission of long-term emotional states merited further study.

Susceptible-Optimistic-Susceptible (SOS) and Susceptible-Pessimistic-Susceptible (SPS)

By the same token, Liu, Zhang, and Lan (2014) extended the SISa framework to model social contagion or *sentiment*. They proposed modelling two infectious states rather than one, as observed in real-life sentiment with positive (optimistic) and negative (pessimistic) states. In treating optimism and pessimism as contagious states, they proposed two processes to describe sentiment contagion dynamics: Susceptible-Optimistic-Susceptible (SOS) and Susceptible-Pessimistic-Susceptible (SPS).



Figure 3.4: Diagram of Susceptible, Optimistic, Susceptible, Spontaneous (SOSa) and Susceptible, Pessimistic, Susceptible and Spontaneous (SPSa) Model with Transitional Rates

The dynamics of SOSa-SPSa model are shown in Figure 3.4. The q_O and q_P parameters are probabilities of a Susceptible individual becoming Optimistic or Pessimistic, respectively. And g_O and g_P are recovery rates from either the optimistic or pessimistic state to susceptible. They

assumed that the process of transition to the optimistic and the pessimistic are independent, and they have fixed population sizes. Using the estimated data from Hill et al. (2010) on the Framingham Heart Study, they analysed this process of sentiment contagion using numerical and agent-based simulations. They found that the results of the SOSa-SPSa model matched the SISa experimental data and they were able to demonstrate that the probability of spontaneous infection or infection through contact would increase with the number of optimistic and pessimistic individuals, but would decrease with the probability of recovery back to susceptible.

There is a vast range of compartmental models, ranging from the most simple frameworks to complex frameworks¹. Even the most simple of these models have produced accurate representations of real-world dynamics and successful forecasting measures (Guan et al. 2020; Lin et al. 2020; Siegenfeld and Bar-Yam 2020; Zhang, Feng, et al. 2022). The popularity of compartmental models in part may be due to this very simplicity that allows modellers to estimate disease behaviour using a small number of parameters (Lourenço et al. 2020; Weissman et al. 2020). A further advantage of compartmental modelling is its adaptability; areas of applications continue to grow, from economics and psychology (Liu, Wu, and Zhu 2007; Øverby, Audestad, and Sza-lkowski 2023; Szalkowski and Mikalef 2023) to computer science (Piqueira et al. 2008; Shahrear et al. 2018). Adaptability refers to the addition of compartments given the object of study. Compartmental modelling offers the advantage of aggregating information from both local and system scale models. Furthermore, compartmental models allow multi-scale modelling with low computational time compared to other methods (Jourdan et al. 2019).

Be that as it may, compartmental models are not without their limitations. Although the simplicity of compartmental models makes them easy to compute, they oversimplify complex infection processes (Sharov 2020). For example, the basic SIR model does not account for the latent period between when an individual is exposed to a disease and when that individual becomes infected and contagious, whereas extensions of the SIR model, such as the SEIR model, accommodate for this parameter (Clancy and O'Neill 2008). Further, compartmental models have limiting assumptions about the population (Roberts et al. 2015; Dhar 2020). They assume homogeneous mixing,

¹See Tang, Zhou, et al. (2020) for a comprehensive review of compartmental models.

meaning all individuals share an equal probability of becoming infectious following contact with one another. This may not reflect the dynamics evident in real life where infection may depend on social networks, individuals would then have different propensities of becoming infectious as the result of a series of contributing factors (Brauer 2008).

To model emotional contagion using compartmental models remains particularly challenging as there exists no widely accepted definition for emotional contagion (Hernandez-Lallement, Gómez-Sotres, and Carrillo 2022). Moreover, the adaptability and choice that compartmental models offer may result in modellers producing discordant results. During the COVID-19 pandemic, the results of SIR models were compared with network transmission models (Zlojutro, Rey, and Gardner 2019; Jewell, Lewnard, and Jewell 2020), to the Institute for Health Metrics and Evaluation's COVID-19 pandemic model based on fitting curves to empirically observed data (Murray 2020). Where different modelling approaches using the same data, produce qualitatively different results it is likely due to differences in underlying assumptions. It is crucial then to consider which of the assumptions are valid explanations of disease dynamics. It is also possible that the data used in these models are insufficient to draw a reliable conclusion. Nevertheless, no model will accurately predict the future but good models should provide approximation sufficient to inform public policy (Tolles and Luong 2020).

3.4.2 Emotional Contagion, Agent-Based Models and Heterogeneity: a discussion

The objective of this section is to present a selection of theoretical frameworks that could be used to develop a case study ABM to investigate heterogeneity in later chapters. Of the many approaches to modelling complex systems that exist, this study models emotional contagion using the familiar dynamics of pathogenic contagion. This is because traditional epidemiology techniques and assumptions, such as compartmental models, have an extensive range of applications and long-standing history (Hethcote 2000; Barrat, Barthélemy, and Vespignani 2008; Rock et al. 2014; Pastor-Satorras et al. 2015; Billah, Miah, and Khan 2020; Øverby, Audestad, and Szalkowski 2023). Furthermore, in the study of complex systems, compartmental models are an established type of system dynamics model (Jourdan et al. 2019).

Compartmental models can be visualised easily, showing all compartments (e.g., individuals in a susceptible or panicked state), flows between states, and feedback loops controlling the flow of panic (Ackley et al. 2017). It is just as simple to express the model using ordinary differential equations (ODE) (Bassingthwaighte et al. 2012). Although they are simple to construct they are often hard to solve analytically (Sterman 2010; Morecroft 2015). Even still, compartmental models allow modellers to experiment with different assumptions and investigate the effect change of system parameters may have on the system dynamics. Compartmental modes are adaptable which means modellers choose which details to include: for example, they tend to include details on disease stages but exclude stochasticity and heterogeneity. It has been proposed that excluding elements of heterogeneity has a larger effect on forecasting the epidemic trajectory, estimating the final epidemic size, and analyzing the impact of interventions (Siegenfeld, Kollepara, and Bar-Yam 2022).

Traditional deterministic compartmental models assume homogeneous mixing, which proposes each individual shares the same probability of contact with all of the others in the population (Keeling and Rohani 2008). Yet, there is a growing consensus that the homogeneous mixing assumption does not hold in the real world because heterogeneity can emerge from numerous sources (Rodríguez and Torres-Sorando 2001), such as age (Brauer and Watmough 2009; Kim, Kang, and Lee 2022), sex (Worden, Porco, et al. 2017; Razak and Zamzuri 2021), susceptibility to disease (Smilkov, Hidalgo, and Kocarev 2014; Yan and Yuan 2020), position in space and the activities and behaviours of individuals (Goscé, Barton, and Johansson 2014; Viguerie et al. 2021), and many others (Bansal, Grenfell, and Meyers 2007). Scientists have continued to develop different approaches to model these various sources of heterogeneity, but it is no easy task.

Compartmental models have been developed to accommodate different objects of study (Kong, Duan, et al. 2022). For example, to study heterogeneity in host contact rates at the population level scientists modified the infection term of the homogeneous mixing compartmental models (Liu, Hethcote, and Levin 1987; Hochberg 1991; Stroud et al. 2006). Other studies have gone further by dividing the compartments into multiple subgroups with similar behavioural characteristics such as risk (May and Anderson 1988) and demography (Schenzle 1984; Babad et al. 1995). In recent

developments in complex network research, a subset has examined the effects of the heterogeneous contact structure on disease spread in networks (Keeling and Eames 2005; Danon et al. 2011).

Alongside the above, there is rapid development in the area of modelling of infectious diseases heterogeneously using ABMs (Dunham 2005; Chen and Xu 2006; Roche, Drake, and Rohani 2011; Hunter, Mac Namee, and Kelleher 2018; Gomez et al. 2021). These models represent heterogeneity through the individual attributes and behaviours (Ajelli et al. 2010; Doussin, Adam, and Georges 2021). Other researchers are working to close the gap between traditional compartmental models and ABMs (Keeling 2005; Roy and Pascual 2006; Aparicio and Pascual 2007; Kong, Wang, et al. 2016).

In light of the above, the rationale for modelling emotional contagion using ABMs over other modelling approaches can be summarised into the following (Smith et al. 2018): *1*) ABMs represent stochasticity often excluded from mathematical modelling of infectious diseases, it allows for an examination of disease dissemination in small or large populations (Maude et al. 2009), *2*) ABMs can be used to produce high-resolution spatial simulations (Raimbault et al. 2020) and *3*) ABMs can capture heterogeneities in individual characteristics (Yu and Bagheri 2020). Therefore, the compartmental model approach specifically the SISa framework, will be used to build the case study ABM in Chapter 4. In addition to this, the SISa framework will be expressed in an ODE model which will be used in this investigation of heterogeneity in Chapter 6.

3.5 Summary - Understanding Contagion

To build a contagion case study model, a theoretical and empirical understanding of collective behaviour is crucial. This chapter begins with an outline of various definitions and forms of collective behaviour, followed by some proposed theories. One of these theories described collective behaviour as a contagion, proposing that it is usually emotionally driven and borne from irrationality. An extension of contagion theory is social contagion theory, which describes collective behaviour as the spread of affect (emotional contagion) and behaviour (behavioural contagion) between participants. Within social contagion theory, emotional contagion is defined as the transmission of emotion between individuals. To model emotional contagion, this chapter considers the

use of compartmental models. Although compartmental models have some limitations, their structural simplicity makes it straightforward to develop into an agent-based model. The adaptability of compartmental models will also allow for modifications as needed to investigate the impact of heterogeneity. The SISa framework described above will be used to build the case study model in Chapter 4.

Chapter 4

Modelling Contagion: An Agent-Based Model

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4.7	Summary - Modelling Contagion

4.1 Chapter Overview

Chapter 3 presented a range of potential underlying theories all of which were suitable frameworks to formulate the case study model, particularly the emotional contagion theorems. This chapter will present a simple agent-based model based on the Susceptible-Infected-Susceptible-Spontaneous (SISa) model framework, which will serve as a case study or a tool to investigate heterogeneity in subsequent chapters. In the wake of COVID-19 and the influx of truly significant impactful

studies using compartmental models, the one presented here should be considered no more than a toy model for illustrative purposes. This chapter is organised as follows: Section 4.2 will present the case study agent-based model using the overview design concepts and details (ODD) protocol outlined by Grimm, Berger, DeAngelis, et al. (2010) to describe the systems processes most appropriately. Section 4.3 will explore the case study model configurations and results to investigate the system dynamics. Section 4.4 and Section 4.5 presents the sensitivity analysis results and the justifications for fixing parameter values. Finally, section 4.6 introduces an ordinary differential equation (ODE) model based on the SISa framework, which will be used in subsequent chapters to demonstrate the potential impact of modelling heterogeneity in ABMs.

4.2 ODD Protocol

4.2.1 Purpose

The case study model proposed here was created to simulate the process and spread of emotional contagion, specifically panic within an agent population¹. Figure 4.1 presents the SISa framework used to design and build the model. Given the simplicity and flexibility of the framework, it serves as an adequate method to compare and examine homogeneous and heterogeneous populations.

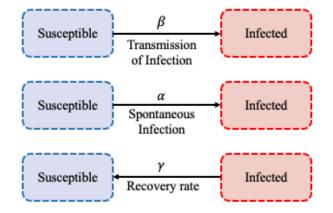


Figure 4.1: SISa framework (Hill et al. 2010, p.3828)

Figure 4.1 summarises the transmission of emotional contagion into two states and three pro-

¹Code for this model can be found on GitHub, here

cesses. Agents can occupy one of two states by the end of each time period (iteration): they are either susceptible or infected. There are three processes through which an agent can move between each state:

- Inter-agent infection rate: a transmission rate of infection to susceptible contacts, denoted here as β .
- Background rate of infection: the constant spontaneous rate of infection that exists within the population, transmitting the infection to a susceptible agent regardless of the state of their contacts, referred to as α .
- **Recovery rate:** the rate of recovery from the infected to susceptible state, independent of the state of their contacts, known as γ .

The processes outlined above are the model attributes and variables used to create the case study.

4.2.2 State Variables and Scales

The case study model is comprised of two configurations: homogeneous and heterogeneous. Both configurations share the same fundamental model and Agent Parameters and processes. In the homogeneous configuration, all agents share the same Agent parameter values; heterogeneity is then introduced through the dividing of agents into groups, where agents in the same group share the same parameters, but agents in different groups have different parameters.

Table 4.1 summarises the parameters and values used to initialise both configurations. Parameter values were chosen arbitrarily for the purpose of model exploration, as a thorough understanding of model dynamics is essential.

There are two broad types of parameters: model-specific and agent-specific parameters. Model Parameters are user-specified inputs that construct the attribute-based environment; these inputs are external and are fixed in both configurations so as not to impact the model results. Agent Parameters are user-specified inputs that construct the agent population of which changes would directly impact model results. The Model Parameters are integers: the Number of Agents, Iterations (Time), Single Instances and Multiple Instances. Agent Parameters are: Alpha (α), Beta (β)

ABM Parameters			
	Homogeneous Config.	Heterogeneous Config.	
Parameter	Value	Value	
Number of Agents	10-1000	10-1000	
Iterations (Time, t)	t	t	
Single Instance	1(t)	1(t)	
Multiple Instances	100(t)	100(t)	
Number of Agent Groups	1	N	
Alpha (α)	0.1	0.1	
Beta (β)	0.386	β_N	
Gamma (γ)	0.2	0.2	

and Gamma (γ) which are rates between 0-1, and Number of Agent Groups.

Table 4.1: Overview of parameters and default values of the panic model

Unless later specified, the parameter values outlined above are to be considered the default or standard for all subsequent experiments. As mentioned previously, heterogeneity will be presented formally through an introduction of Agent Groups, where the Number of Agent Groups = 1 refers to the homogeneous configuration and in the heterogeneous configuration N = (1, 2, 3, ..., N) denotes the number of groups within the whole population (Number of Agents); each Group is assigned a unique Beta (β), where Alpha (α) and Gamma (γ) are be held constant. Thus, β_N where N = (1, 2, 3, ..., n) denotes the number of groups. Further, each Group would have an equal Number of Agents. Similarly, Iterations (Time, t) refers to the length of one simulation, which is a standard t = 100. Single and Multiple Instances refer to the number of simulations: where 1(t) refers to one simulation and 100(t) refers to an average of over 100 simulations.

Lastly, to ensure reproducibility and consistency in the comparative study of model configurations, prior to initialising parameters a random seed was set. Random seeds are stored to ensure that model results are reproducible.

4.2.3 Process Overview and Scheduling

As previously outlined, the case study model is comprised of three simple processes based on the SISa framework. The model operates using a predetermined number of Iterations t, and at each step, agents occupy one of two states: susceptible or infected.

Figure 4.2 illustrates the entire model process. The parameters of which the model is initialised are user-specific and thus are exogenous; agents use the Agent Parameters, α and or β , to form a Likelihood, \mathcal{L} , of becoming panicked (or infected). Likelihoods must be greater than 0 but cannot exceed 1, in other words, $0 < \mathcal{L} \leq 1$. All agents begin in a susceptible state and given their likelihood, they can become infected with panic or avoid infection entirely. Agents evaluate whether to change state once per iteration and do so in no particular order. And once panicked, agents can recover or remain infected. Model processes are the same in both model configurations; this process repeats until the model satisfies the specified number of iterations.

As part of an agent's assessment of their condition, they compare their state to that of another randomly chosen Agent; the former agent can be referred to as Agent_A and the latter agent as Agent_i. When constructing their likelihood of infection Agent_A would account for the state of Agent_i in the previous iteration. Therefore, if Agent_i were susceptible, Agent_A would construct their likelihood only using the background rate of infection i.e., $\mathcal{L} = \alpha$. If Agent_i were infected, Agent_A would construct their likelihood using α and β i.e., $\mathcal{L} = \alpha + \beta$. To recover, the agent likelihood is $\mathcal{L} = \gamma$.

To recapitulate, when the agent population are homogeneous they construct their likelihood using the same α , β values; when the agent population are heterogeneous they construct their likelihood using α which is fixed, and an exclusive β unique to their Agent Group. To formally switch states, agent likelihood and recovery rate must satisfy the following condition: $\mathcal{L} > r$, where r is a randomly generated number.

4.2. ODD PROTOCOL

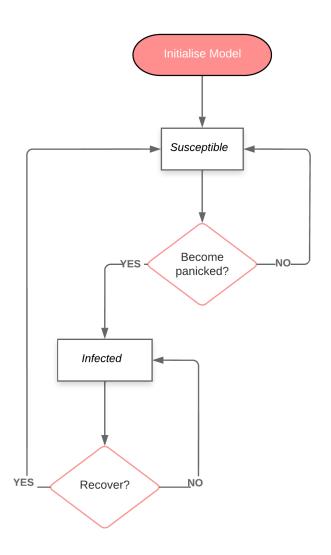


Figure 4.2: Panic ABM Full Process Overview and Agent Lifecycle

4.2.4 Design Concepts

The most important design concepts of the model are outlined in Table 4.2.

4.2. ODD PROTOCOL

EmergenceLarger scale population dynamics emerge from the behaviour of the individual agents. All agent behaviours are initiated through a rule set i.e., how agents compute their individual likelihoods and when agents should switch states from Susceptible to Panicked (Infected).AdaptationThe Panic ABM does not model adaptation, although extensions of the	
Emergence i.e., <i>how</i> agents compute their individual likelihoods and <i>when</i> agents should switch states from Susceptible to Panicked (Infected). The Panic ABM does not model adaptation, although extensions of the	
i.e., <i>how</i> agents compute their individual likelihoods and <i>when</i> agents should switch states from Susceptible to Panicked (Infected). The Panic ABM does not model adaptation, although extensions of the	
The Panic ABM does not model adaptation, although extensions of the	
The Panic ABM does not model adaptation, although extensions of the	
model that include adaptation could be designed.	
At an individual agent level, fitness is measured by agents likelihood.	
Fitness Although likelihoods are bound between 0-1, the actual value does not	
determine whether they become infected or remain susceptible.	
Prediction Agents hold no predictive abilities, they cannot predict future outcomes.	
Agents have a list of the number of panicked agents at all times which	
updates at each new time-step.	
Agents interact indirectly on a local level. At a local level, the state of an Interaction	
infected agent can affect the state of other susceptible agents.	
A randomly generated number is used to become panicked and recover	
Stochasticity from infection. The agent order and the comparative agent i.e., $Agent_i$, are	
also randomised. A random seed makes a specific stochastic run reproducib	ole.
The agent population is divided by the specified number of agent groups.	
Collectives Each agent group has a specific beta value that agents adopt. Agents	
can observe others within the same group, but they do not interact directly.	
Observations are a graphical display of the number of infected agents	
through time. For model exploration and sensitivity analysis, the number Observation	
of infected for each beta parameter and the cumulative distribution of the	
number of infected is recorded.	

Table 4.2: Design Concepts Checklist

4.2.5 Initialisation

To initialise the case study model, all the ABM Parameters listed in Table 4.1 have to be determined by the modeller.

The Model Parameters: Number of Iterations, Number of Agents, and Single and Multiple Instances, were to be held constant or fixed for the benefit of comparative study and scientific integrity. The user would then have to determine whether they are assuming heterogeneity or homogeneity by specifying a Number of Agent Groups. Agents are then created based on the specification. To model homogeneity, the Number of Agent Groups cannot exceed one, as this parameter value predetermines the number of β values to be created and incorporated into the ABM. When the Number of Agent Groups is greater than one, the total agent population would be divided by this value, and each Group is designated a unique β value.

The agent parameter value: α , β and γ can be chosen arbitrarily or better informed by sensitivity analysis or expertise. In the homogeneous configurations, α , β and γ values are fixed. In heterogeneous configurations, α and γ are fixed whereas β varies.

Initialisation, regardless of the user's choice of configuration, the process remains the same and does not change.

4.2.6 Input

The dynamics of this case study ABM are informed only by agent attributes or parameters. Agents do not interact with an environment that changes over space and time, the agent environment is extremely abstract. The only dimensions captured within this model are iterations, which are predetermined by the modeller at the point of initialisation.

4.2.7 Sub-models

The panic ABM is a simple model which does not include any sub-models.

4.3 Model Exploration

This case study model consists of the parameters outlined in Table 4.1. As previously mentioned, the Agent Parameters were formed based on the three model processes outlined in the previous section, α , β and γ with the addition of the Number of Agent Groups, the heterogeneity indicator. Model Parameters are assigned at the point of initialisation, and unlike the Agent Parameters, are fixed regardless of the user's choice of configuration. This section will explore the relationship between the ABM input and output, namely, the effect that Agent Parameters have on the Number of Infected Agents in the homogeneous and heterogeneous configurations.

All agents begin in a Susceptible state i.e. free of any infection, which in this case, means they are free of panic. In time, given their likelihood of infection, agents develop a propensity to become panicked and to assume an Infected state. Agents interact indirectly through the observation of Agent_i present state, where Agent_i is randomly selected from the population. If Agent_i is Infected, that agent's probability of becoming infected increases. Agents recover in the same fashion, given their probability informed by γ , a fixed rate.

The following sections will present the homogeneous and heterogeneous configurations and provide insights into the system dynamics.

4.3.1 Homogeneous Configuration

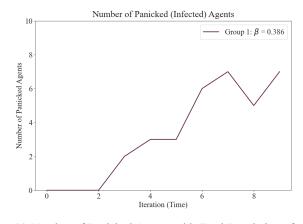
The values used to initialise the homogeneous configuration were outlined in Table 4.3 and were chosen arbitrarily. To begin with, the Agent Parameters α , β , γ and Number of Agent Groups were fixed, whilst the Number of Agents and Iterations varied for the specific purpose of evaluating their impact on the Number of Infected Agents or model output.

Homogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	10-1000	
Number of Iterations (Time, t)	10-1000	
Number of Agent Groups	1	
α	0.1	
β	0.386	
γ	0.2	

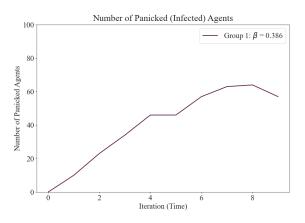
Table 4.3: Homogeneous Configuration Parameter Values

Figure 4.3 illustrates the Number of Infected with total populations of 10, 100 and 1000 agents, over 10 iterations. Given the method by which agents construct their likelihoods, it seems that as long as α and or $\beta > \gamma$, there would be an initial increase in the Number of Infected Agents that would eventually reach a constant rate or steady state.

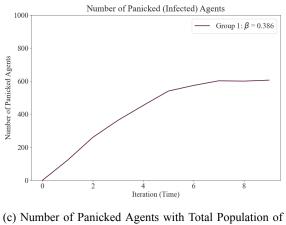
And as expected, Figure 4.3 satisfies this assumption. As the Number of Agents increased from 10 to 100 (Figure 4.3b) and 1000 (Figure 4.3c), the Number of Infected exhibited a less sporadic, fluctuating nature but it will become clear that the simulations reach a "steady state" toward the latter stages.



(a) Number of Panicked Agents with Total Population of 10 Agents



(b) Number of Panicked Agents with Total Population of 100 Agents



(c) Number of Panicked Agents with Total Population of 1000 Agents

Figure 4.3: Number of panicked agents with an increasing agent population over 10 iterations

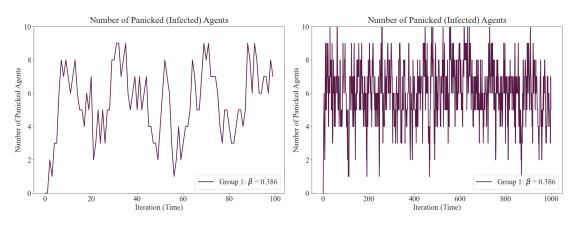
4.3. MODEL EXPLORATION

To explore the effects of Time on the Number of Infected, the model was simulated over 100 and 1000 Iterations, see Figure 4.4. In comparison to Figure 4.3, in Figures 4.4a and 4.4b increasing the Number of Iterations whilst the agent population is kept small, introduced a sporadic, fluctuating nature. With fewer agents, there seemed to be a larger variance in the Number of Infected as illustrated by the extreme peaks and troughs.

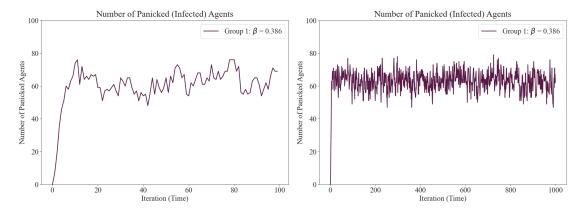
When increasing the Number of Agents to 100, as shown in Figures 4.4c and 4.4d, the variance of the Number of Infected shrinks. Though there was still some irregular oscillation, there were far less observable extremes. Similarly, Figures 4.4e and 4.4f present the results of 1000 agents over 100 and 1000 iterations, respectively. An immediate observation was how little variance was present in the dynamics of the Number of Infected, though there was still some noise or oscillation.

Moreover, when considering the stationary distribution and how it could be achieved, there were three Model Parameters that became the subject of focus: Number of Agents, Iterations and Instances (Single and Multiple)². Figure 4.5 presents the effect of each Model Parameter.

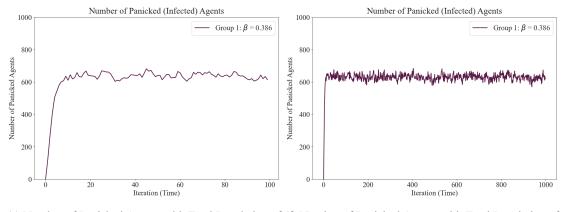
²For more on Single and Multiple Instances, see Table 4.1.



(a) Number of Panicked Agents with Total Population of (b) Number of Panicked Agents with Total Population of 10 Agents10 Agents

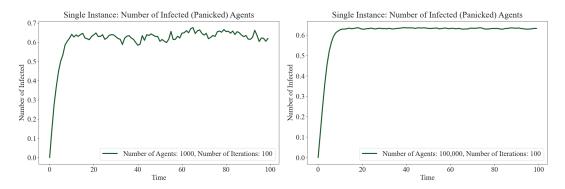


(c) Number of Panicked Agents with Total Population of (d) Number of Panicked Agents with Total Population of 100 Agents100 Agents

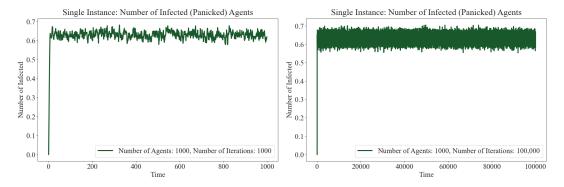


(e) Number of Panicked Agents with Total Population of (f) Number of Panicked Agents with Total Population of 1000 Agents1000 Agents

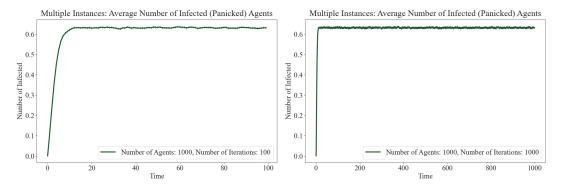
Figure 4.4: Number of panicked agents with an increasing agent population over 100 and 1000 iterations



(a) Single Instance: Number of Panicked Agents with (b) Single Instance: Number of Panicked Agents withTotal Population 1000 over 100 IterationsTotal Population 100,000 over 100 iterations



(c) Single Instance: Number of Panicked Agents with (d) Single Instance: Number of Panicked Agents withTotal Population 1000 over 1000 IterationsTotal Population 1000 over 100,000 Iterations



(e) Multiple Instances: Average Number of Panicked (f) Multiple Instances: Average Number of Panicked Agents with Total Population 1000 and 100 Iterations Agents with Total Population 1000 and 1000 Iterations over 100 Model Instances over 100 Model Instances

Figure 4.5: The effect of Number of Panicked Agents, Number of Iterations and Model Instances has on Stochasticity

Figures 4.5a and 4.5b were model results over a Single Instance and 100 iterations; the visualisations demonstrate that increasing the Number of Agents from 1000 to 100,000 approximately the same steady state is reached. Figures 4.5c and 4.5d allude to the same findings, albeit the behaviours present differently. Showing that increasing the Number of Iterations has no observable effect on the Number of Infected; that being said, it is indicative of potentially having reached a steady state. Although there are some observable peaks and troughs, the variance is unchanged through time, it remains stationary.

And finally, when the ABM was simulated over Multiple Instances, as in Figures 4.5c and 4.5d, the Number of Infected denotes the *Average* specifically over 100 instances. In contrast to Figures 4.5a and 4.5b where the Number of Iterations increased from 100 to 1000, the variance mirrors behaviours exhibited when increasing the Number of Agents (see, Figures 4.5a and 4.5b). This suggests that simulating the ABM with a larger Number of Agents in a Single Instance has a similar smoothing effect on the Number of Infected, to the *Average* Number of Infected from a smaller Number of Agents and Number of Iterations. Leading on from this, as there are no observable or unexpected deviations, there is a sensible degree of confidence and certainty that can be assumed by the user when considering the performance of this case study model.

To supplement the above, Ordinary Differential Equations (ODE) will be used to reproduce the ABM scenario illustrated in Figure 4.5e later in this Chapter. The purpose of this comparison will be to investigate whether an inherently deterministic model (ODE) and stochastic model (ABM) could ever match. Figure 4.6 presents the Number of Infected, where the ODE and ABM were initialised with the same Number of Agents (1000) and Number of Iterations (100). As the ABM was inherently stochastic, the *Average* Number of Infected over Multiple Instances (100) was used, rather than over a Single Instance. From this model comparison, there is evidence of some convergence, as both exhibit qualitatively similar dynamics.

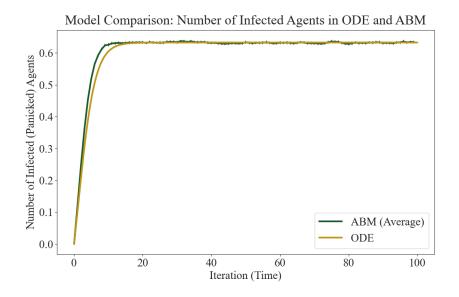


Figure 4.6: Model Comparison: Deterministic ODE and Stochastic ABM

4.3.2 Heterogeneous Configuration

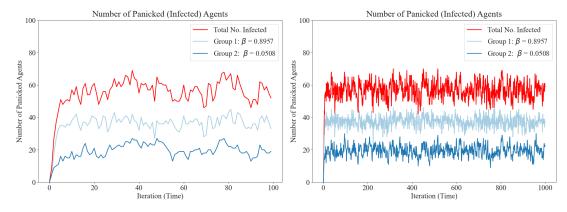
Heterogeneity is introduced through the Number of Agent Groups parameter, first outlined in Table 4.1. Whereby, the Number of Agents would be divided by the Number of Agent Groups. Each Group would then be assigned a unique β value which was chosen arbitrarily; where α and γ were held constant. To first present this configuration, extreme values of β were selected to investigate whether the dynamics of high and low infectious rates could be observable in model output. Table 4.4 outlined the parameter values used to initialise the heterogeneous configuration of the ABM. The exploration began by increasing the Number of Agent Groups = 2.

Heterogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	10-1000	
Number of Iterations (Time, t)	10-1000	
Number of Agent Groups	2	
α	0.1	
$eta_{ ext{Group 1}}$	0.8957	
$\beta_{ m Group}$ 2	0.0508	
γ	0.2	

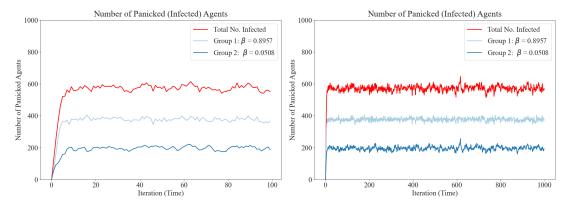
Table 4.4: Heterogeneous Configuration Parameter Values

The Number of Infected with total populations of 10, 100 and 1000 agents over 10 iterations can be found in Appendix A; Figure A.1 presents the same smoothing effects as it previously observed in Figure 4.3. Moreover, Figure 4.7 illustrates the Number of Agents and Number of Iterations at 100 and 1000, which reproduce similar dynamics seen in Figure 4.4. When the Number of Agents is held constant at 100, but the Number of Iterations increases from 100 (Figure 4.7a) to 1000 (Figure 4.7b), the Number of Infected presents a familiar sporadic, oscillating nature.

4.3. MODEL EXPLORATION



(a) Number of Panicked Agents with Total Population of (b) Number of Panicked Agents with Total Population of 100 Agents over 100 Iterations100 Agents over 1000 Iterations



(c) Number of Panicked Agents with Total Population of (d) Number of Panicked Agents with Total Population of1000 Agents over 100 Iterations1000 Agents 1000 Iterations

Figure 4.7: Number of panicked agents with increasing agent population over 100 and 1000 iterations

When the Number of Agents increased and fixed at 1000, but the Number of Iterations was increased from 100 (Figure 4.7c) to 1000 (Figure 4.7d), the variance of the Number of Infected is significantly smaller and there are less observable extremes; but the overall dynamics of the model do not diverge from what was previously seen. Furthermore, $\beta_{\text{Group 2}} = 0.0508$ has the smallest proportion in the Number of Infected; be that as it may, the steepness of each slope is not as clear.

Another area of interest in the exploration of the heterogeneous configuration was: to investigate

whether the proportion of the Number of Agents within each Group, would impact the nature of the Number of Infected. Figure 4.8 presents these results but to comprehend the behaviours, the dynamics of the heterogeneous configurations were expressed algebraically.

The Number of Agents or total agent population could then be expressed as:

$$N = N_1 + N_2, (4.1)$$

where N_1 was the Number of Agents in Group 1 and N_2 was the Number of Agents in Group 2 respectively. Each Group were assigned their own unique β values in this case:

$$N_1 = \beta_{\text{Group 1}} = 0.8957$$

 $N_2 = \beta_{\text{Group 2}} = 0.0508.$

Eqn. (4.1) implies,

$$1 = \frac{N_1}{N} + \frac{N_2}{N}$$

where 1 denotes the total agent population.

Therefore, the proportion of the Number of Agents in Group 1 could be defined as the following:

$$\theta_1 = \frac{N_1}{N},\tag{4.2}$$

where $\theta_1 = [0, 1]$ and expresses a proportion of agents between 0% - 100%.

Given Eqn. (4.2), it stands that:

$$\frac{N_2}{N} = 1 - \theta_1.$$

Then,

$$\hat{\beta} = \frac{N_1}{N} \beta_1 + \frac{N_2}{N} \beta_2 = \theta_1 \beta_1 + (1 - \theta_1) \beta_2$$
(4.3)

In essence, Figure 4.8 illustrates how varying the proportion of the Number of Agents within each Group, would impact the nature of the Number of Infected. For reference, the parameter values used in initialising the ABM for this investigation are in Table 4.5.

To begin, the *Average* Number of Infected was approximated over 100 instances in both the homogeneous and heterogeneous cases. The homogeneous cases referred to the scenarios where 100% of the Number of Agents were either Group 1 or Group 2, respectively; and the heterogeneous cases referred to the scenarios where the Proportion of the Number of Agents allocated to either Group 1 or Group 2, decreased and increased respectively.

In Figure 4.8, where 100% of the Number of Agents were allocated to Group 1, the *Average* Number of Infected was depicted by the static blue line. And when, 100% of the Number of Agents were allocated to Group 2, the *Average* Number of Infected was depicted by the static magenta line. As one would expect, Group 1 presented a higher steady-state than Group 2, which reflects the size of their β values.

In addition to the above, particularly in reference to the scenario where 100% of the Number of Agents were allocated to Group 2, the *Average* Number of Infected at each incremental +1%change is captured by the increasing grey bars. This insinuates that as the Number of Agents in the simulation increases, so does the Fraction of Infected.

As the Number of Agents in Group 1 decreases in increments of 1%, the Number of Agents in Group 2 increases by the same proportion. This negative relationship is captured by the green dashed line, which is the Heterogeneous Total Infected Fraction. Therefore, it can be reasoned that the proportion of the Number of Agents in each group is what matters most, as the changes in Total Infected Fraction reflect the β of the group with a larger fraction of the Number of Agents, not the group with the highest β .

Heterogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	100	
Number of Iterations (Time, t)	100	
Multiple Instances	100(t)	
Number of Agent Groups	2	
α	0.1	
$\beta_{ m Group 1}$	0.8957	
$\beta_{ m Group \ 2}$	0.0508	
γ	0.2	

Table 4.5: Parameters for the investigation of varying Proportion of Agents in Agent Groups

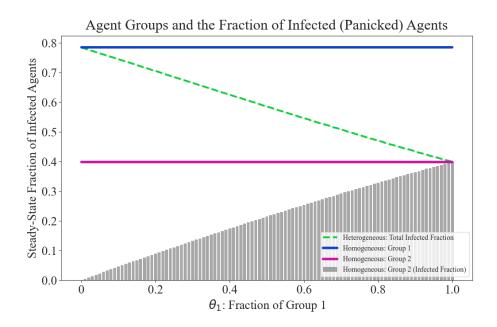


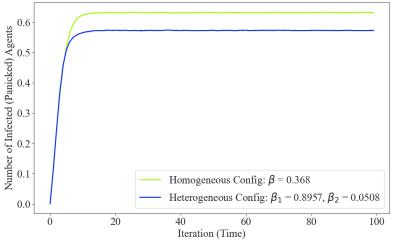
Figure 4.8: The impact of Agent Groups (Heterogeneity) on the dynamics of the Number of Infected (Panicked) Agents

4.3.3 Homogeneous and Heterogeneous Configuration Comparison

Figure 4.9 compares the dynamics of *Average* Number of Infected for Homogeneous and Heterogeneous configurations, where Table 4.6 contains the parameter values used to initialise each model.

ABM Parameters			
	Homogeneous Config.	Heterogeneous Config.	
Parameter	Value	Value	
Number of Agents	1000	1000	
Iterations (Time, t)	100	100	
Multiple Instances	1000(t)	1000(t)	
Number of Agent Groups	1	2	
Alpha (α)	0.1	0.1	
Beta (β)	0.386	0.8957, 0.0508	
Gamma (γ)	0.2	0.2	

Table 4.6: Configuration Comparison: Agent and Model Parameter Values



Model Comp: Number of Infected in Homogeneous and Heterogeneous Config

Figure 4.9: Comparison of the Number of Infected in Homogeneous and Heterogeneous Configurations. The dynamics of the homogeneous and heterogeneous configurations were compared. In the homogeneous case where $\beta = 0.386$, the *Average* Total Number of Infected was 62. In the heterogeneous case, where $\beta_1 = 0.8957$ and $\beta_2 = 0.0508$, the *Average* Total Number of Infected was 56.

Figure 4.9 indicates that both configurations follow similar dynamics and there are no unexpected deviations. However, even when α and γ are held constant, the proportion of the *Average* Number of Infected is significantly higher in the Homogeneous Configuration. A possible explanation for this may relate to the investigation of Agent Groups in the previous section: in that, only 50% of the agents have a higher β , these are agents in Group 1 of the Heterogeneous configuration. Agents in Group 2 have a lower infection rate and thus are less likely to become infected. This reduces the Total Number of Panicked agents in the Heterogeneous configuration. To supplement the above, not only does the size of β significantly affect the *Average* Number of Infected, but so does the proportion of the Number of Agents in each group.

On a final note, this comparison suggests a possibility of equivalent homogeneous and heterogeneous models if attention is paid to selecting β values which produce approximate *Average* Total Number of Infected. This exercise suggests that closing the distance of the *Average* Number of Infected between Homogeneous and Heterogeneous Configurations in Figure 4.9 could be achieved by purposefully selecting combinations of β values which reflect approximate *Average* Total Number of Infected values. Though this may be a significant observation from model exploration, the objective of this study is to investigate the impact of the introduction of heterogeneity using this toy model, not to necessarily prove the equivalence between homogeneous and heterogeneous. Be that as it may, an investigation into potential equivalence could be explored in future work.

4.4 Sensitivity Analysis

The previous section explored the dynamics of the homogeneous and heterogeneous configurations of the case study model; however, the values used to simulate the findings were chosen arbitrarily. Thus, it is paramount to conduct further study of the robustness and overall uncertainty of the ABM. In other words: *how different values of* α , β and γ affect the Number of Infected? And with the analysis, Section 4.5 will use it to present the rationale underpinning the fixing of Agent Parameters in subsequent chapters. The aim of this sensitivity analysis³ is to distinguish optimal parameter values based on their effect on model output.

4.4.1 Background Rate Of Infection: α

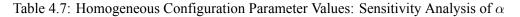
As mentioned previously, as Agent Parameters are rates, they are bound between 0-1 to demonstrate the growth and decline of infection. In this study, α was defined as the background rate of Infection. Thus, α was the constant spontaneous rate of infection that existed within the population, transmitting the infection to a susceptible agent regardless of the state of their contacts. To evaluate the effect of its fluctuations on the Number of Infected, β , γ and all the other ABM parameters were held constant (See Table 4.7). As done earlier, it is assumed that α will have a positive, increasing effect on the Number of Infected.

In Figure 4.10, γ is held constant along rows at 0.25 and 0.75 in the top and bottom rows respectively. Similarly, in Figure 4.10, β is held constant down columns and has the values 0.25 and 0.75 in the left and right columns respectively. Along the y-axis is the *Average* Number of Infected as α increases between 0-1.0. As expected, as α increases, so does the *Average* Number of Infected. And as previously seen, α and or $\beta > \gamma$ continue to determine the steepness of the slope in the *Average* Number of Infected, before reaching a steady state.

The figures in the *top-row* suggest that when γ is small: on the left column, as α increases so does the *Average* Number of Infected. On the right column, where β is high so is the *Average* Number of Infected. But the effect of α is less noticeable. On the *bottom-row*, where γ is high, as α increases as does the *Average* Number of Infected. In both columns, as α and β increase so

³The sensitivity analysis script can be found on GitHub, here.

Homogeneous Config: ABM Parameters	
Parameter	Value
Number of Agents	1000
Number of Iterations (Time, t)	100
Multiple Instances	100(t)
Number of Agent Groups	1
α	0.0-1.0
β	0.025, 0.075, 0.25, 0.75
γ	0.025, 0.075, 0.25, 0.75



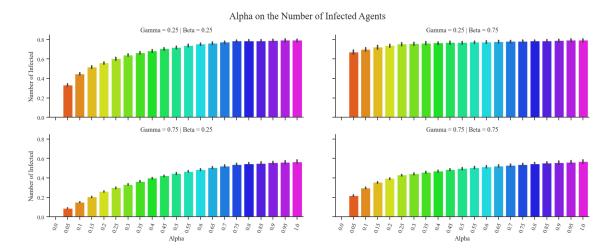


Figure 4.10: Alpha on the Average Number of Panicked Agents (0.0-1.0)

does the *Average* Number of Infected. Though compared to the *top-row*, the *Average* Number of Infected is significantly smaller. Figure 4.11 considers the *Average* Number of Infected when α ranges between 0-0.1, where β and γ are still fixed at 0.25 and 0.75. Here, though smaller, as α increases so does the *Average* Number of Infected. Though this is less noticeable where $\beta = 0.75$ and $\gamma = 0.25$. Compared to Figure 4.10, the comparatively lower α values reflect in the lower *Average* Number of Infected.

Further, Figure 4.12 considers *Average* Number of Infected when α ranges 0-0.001, where β and γ are fixed at 0.025 and 0.075. This Figure suggests, that when α is significantly small there is a variability in its effect on the *Average* Number of Infected. These Figures serve as motivation to keep α between 0.0 - 0.1, as this is when the effect of α is most observable on the *Average* Number of Infected. That being said, where β and γ are too large, the effect of α is less apparent.

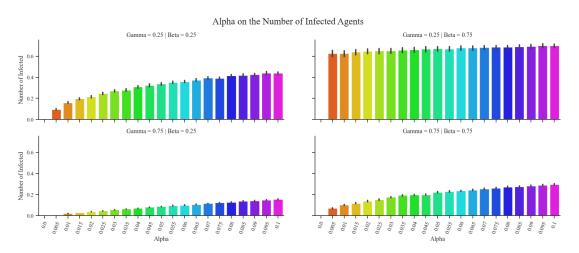


Figure 4.11: Alpha on the Average Number of Panicked Agents (0.0-0.1)

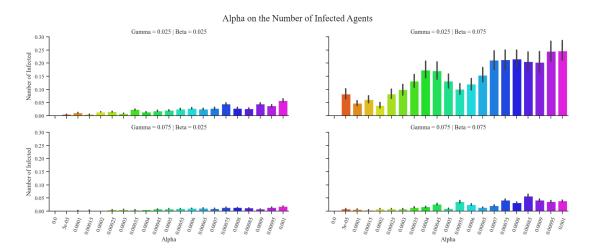


Figure 4.12: Alpha on the Average Number of Panicked Agents (0.0-0.001)

4.4.2 Inter-agent Infection Rate: β

The inter-agent infection rate, β , refers to the transmission rate at which susceptible contacts become infected. The analysis above was repeated to capture the effect of β on the *Average* Number of Infected. Once more the ABM parameters were held constant, see Table 4.8.

Homogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	100	
Multiple Instances	100(t)	
Number of Agent Groups	1	
α	0.025, 0.075, 0.25, 0.75	
β	0.0-1.0	
γ	0.025, 0.075, 0.25, 0.75	

Table 4.8: Homogeneous Configuration Parameter Values: Sensitivity Analysis of β

As assumed with α , β is expected to exhibit similar positive behaviours, in that it should have an increasing effect on the *Average* Number of Infected.

In Figure 4.13, γ is held constant along rows at 0.25 and 0.75 in the top and bottom rows respectively. Similarly, in Figure 4.13, α is held constant down columns and has the values 0.25 and 0.75 in the left and right columns respectively.

Along the y-axis is the *Average* Number of Infected as β increases between 0-1.0. On the *top-row*, the left figure shows, that as β increases so do the *Average* Number of Infected; however, this is effect not evident in the right figure where *Average* Number of Infected remains constant. Likewise on the *bottom-row*, β increasing does not seem to significantly affect *Average* Number of Infected. This Figure suggests that even when β increases particularly when α is high, *Average* Number of Infected remains constant.

4.4. SENSITIVITY ANALYSIS

CHAPTER 4. MOD-ELLING CONTAGION: AN AGENT-BASED MODEL

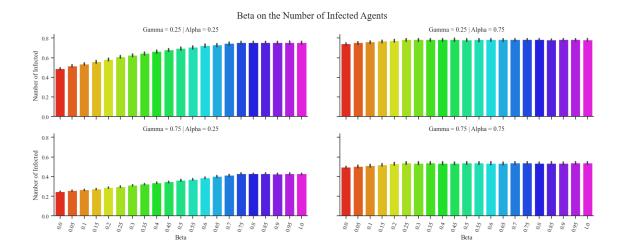


Figure 4.13: Beta on the Average Number of Panicked Agents (0.0-1.0)

Unlike with behaviours exhibited by α when smaller, Figure 4.14 presents β between 0-0.1. And in both *top and bottom-rows*, the behaviour of the *Average* Number of Infected are somewhat identical. There is no observable effect of β as it increases on the *Average* Number of Infected, it actually remains constant. Figure 4.15 presents the case where β ranges between 0.0 - 0.001, and γ and α are fixed at 0.025 and 0.075. The behaviours present mirror those previously seen: as β increases, the *Average* Number of Infected maintains a constant rate and does not vary. These Figures suggest that the effects of β are most noticeable between 0.0 - 1.0, any smaller than its effect becomes practically unobservable.

4.4. SENSITIVITY ANALYSIS

CHAPTER 4. MOD-ELLING CONTAGION: AN AGENT-BASED MODEL

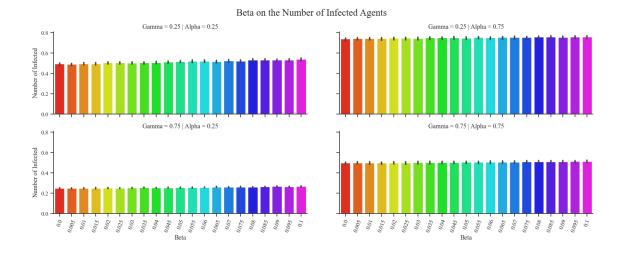


Figure 4.14: Beta on the Average Number of Panicked Agents (0.0-0.1)

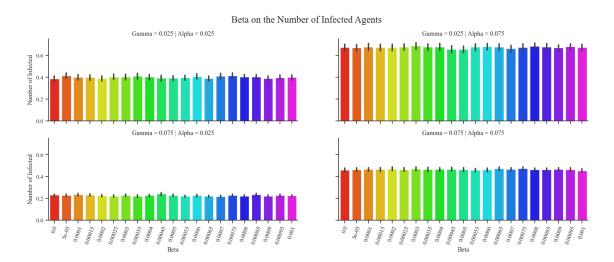


Figure 4.15: Beta on the Average Number of Panicked Agents (0.0-0.001)

4.4.3 Recovery Rate: γ

The rate of recovery, γ , was described as the rate at which infected agents would return to a susceptible state, independent of the state of their contacts. To capture its effect, the experiments above were replicated and the ABM Parameters were held constant (See Table 4.9).

Homogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	100	
Multiple Instances	100(t)	
Number of Agent Groups	1	
α	0.025, 0.075, 0.25, 0.75	
β	0.025, 0.075, 0.25, 0.75	
γ	0.0-1.0	

Table 4.9: Homogeneous Configuration Parameter Values: Sensitivity Analysis of γ

Although γ is non-negative, given its dynamics, it can be assumed that γ will have a negative effect on the Average Number of Infected agents.

In Figure 4.16, β is held constant along rows at 0.25 and 0.75 in the top and bottom rows respectively. Similarly, in Figure 4.16, α is held constant down columns and has the values 0.25 and 0.75 in the left and right columns respectively.

Along the y-axis, as γ increases between 0-1.0 the *Average* Number of Infected decreases. This negative effect observed as γ increases does not change in either *top and bottom-rows*. In Figure 4.17 γ ranges between 0.0-0.1, and as it γ increases, the *Average* Number of Infected still decreases. However, there is a noticeably shallower decline observed in the *Average* Number of Infected.

4.4. SENSITIVITY ANALYSIS

CHAPTER 4. MOD-ELLING CONTAGION: AN AGENT-BASED MODEL

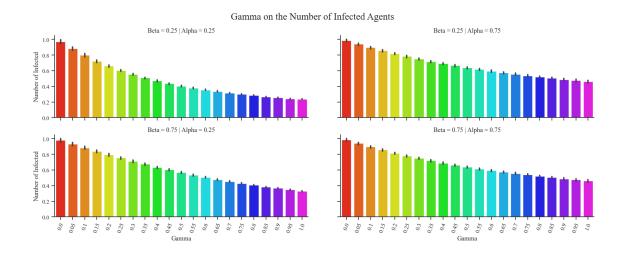


Figure 4.16: Gamma on the Average Number of Panicked Agents (0.0-1.0)

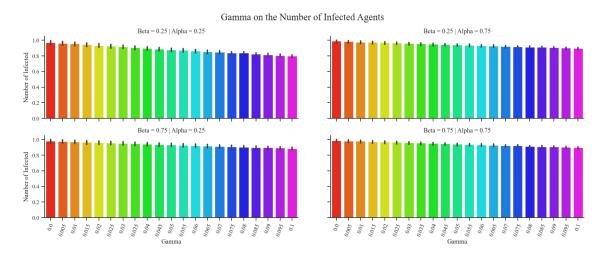


Figure 4.17: Gamma on the Average Number of Panicked Agents (0.0-0.1)

In Figure 4.18 γ spans between 0.0-0.001 and β and α are fixed at 0.025 and 0.075. Here, the *Average* Number of Infected follows similar dynamics observed in Figure 4.14 and Figure 4.15. As, γ increases, there is no observable change in the *Average* Number of Infected, it remains constant. These Figures suggest that the effect of γ on *Average* Number of Infected is most perceptible between 0.0 - 1.0, this serves as motivation to keep γ relatively high.

4.4. SENSITIVITY ANALYSIS

CHAPTER 4. MOD-ELLING CONTAGION: AN AGENT-BASED MODEL

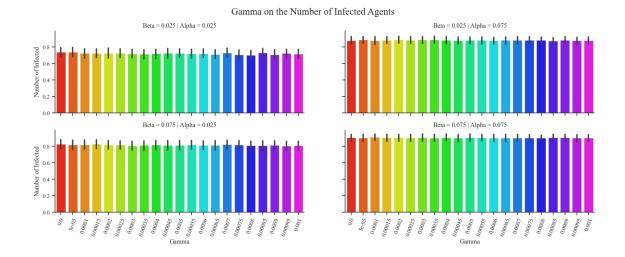


Figure 4.18: Gamma on the Average Number of Panicked Agents (0.0-0.001)

4.5 Parameter Value Selection: Distinguishing Initial Input Values

The sensitivity analysis conducted in the previous section evaluated the parameter space of each Agent Parameter. Thus, it can be utilised to distinguish and justify suitable values for each parameter given research objectives. Furthermore, fixing parameters ensures consistency throughout the remaining chapters. This will be demonstrated by scaling all parameters to show that time yields qualitatively similar results, thus one parameter can be justifiably fixed. In this case, the fixed parameter will be γ , see Figure 4.19.

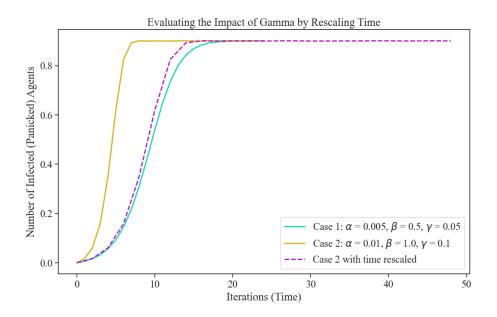


Figure 4.19: Demonstrating the Impact of Gamma by Rescaling Time

Figure 4.19, presents a two-case study and the Agent Parameters used to initialise the models are summarised in Table 4.10. Case 1, depicted by the turquoise-blue line, was simulated with the following values: $\alpha = 0.005$, $\beta = 0.5$, $\gamma = 0.05$. Case 1 presents an initial increasing slope in the *Average* Number of Infected, before eventually reaching a steady-state. In Case 2, depicted by the yellow line, α , β , γ were multiplied by 2; when compared to Case 1, the line is characterised by a comparatively steeper slope. The steeper gradient is the result of a higher likelihood, which then paired with a higher rate of recovery, resulting in the steady-state being reached sooner than in Case 1. By rescaling Time, multiplying t by 2 on Case 2, and is depicted by the purple dashed

Homogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	100	
Number of Iterations (Time, t)	25, 50	
Multiple Instances	100(<i>t</i>)	
Number of Agent Groups	1	
α	0.005, 0.01	
β	0.5, 1.0	
γ	0.05, 0.1	

Table 4.10: Homogeneous Configuration Parameter Values: Effect of γ by Rescaling Time

line. Most interestingly, Case 2 and Case 2 with rescaled Time converge at the same steady-state rates. This Figure shows that qualitatively similar dynamics as the result from rescaled parameters when time is appropriately rescaled. Thus, one of the parameters can be fixed while the other two are varied, since the dynamics resulting from any other combination of parameters will be captured in those considered via an appropriate rescaling. Based on this γ will be fixed at 0.1 hereinafter

Sections 4.4.1 and 4.4.2 presented the interesting dynamics of of α and β , respectively. Both α and β presented an increasing relationship with the *Average* Number of Infected. When α was significantly small, there was more variability in the behaviour of the *Average* Number of Infected; in contrast to β , which proved to have very little variability overall but was most dynamic when α was comparatively smaller. To continue the identification of optimal parameter values, γ was held at 0.1 then α and β were varied between 0.0-0.01 and 0.0-1.0 respectively, Figure 4.20 presents the Average Number of Infected Agents as a Heatmap.

4.5. PARAMETER VALUE SELEC-TION: DISTINGUISHING INITIAL INPUT VALUES

CHAPTER 4. MOD-ELLING CONTAGION: AN AGENT-BASED MODEL

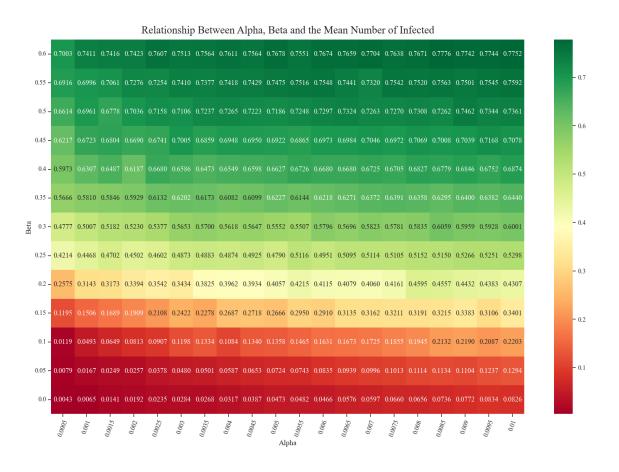


Figure 4.20: Examining the relationship between Alpha, Beta and the Mean Number of Infected Agents

In Figure 4.20, where α is very low then increasing β initially has no effect, but then rather quickly *Average* Number of Infected increases. For larger α values, this effect is evident in lower values of β . Thus, α will be held constant at 0.01. As demonstrated in 4.4.2, where α is large the effect of β becomes imperceptible, which serves as a further motivation to constrain α to comparatively smaller values.

And lastly, when considering β in the Homogeneous Configuration, where $\alpha = 0.01$, any value between 0.0-0.6 would be appropriate. Naturally, as β is a rate, to observe the effect of the interagent infection rate the selected value should be greater than 0. But when introducing Heterogene-

ity, it may be worth considering allocating β values to Agent Groups which are distinctive, so the dynamics of *Average* Number of Infected are comparatively different and effects are distinguishable.

4.6 Modelling Contagion: an ODE Illustration

This section introduces an ODE model based on the SISa framework used to develop the case study ABM. The ODE model only considers a homogeneous population but will be used later in Chapter 6 to propose parameter identification issues as an impact of modelling heterogeneity.

The dynamics of the emotional contagion SISa model can be expressed by the following set of ordinary differential equations,

$$\frac{dI}{dt} = aS + bSI - gI,$$

$$\frac{dS}{dt} = -aS - bSI + gI,$$
(4.4)

where I(t) and S(t) are the number of infected and susceptible agents respectively at time t, b is the transition rate from infected to susceptible, a is the rate of spontaneous infection, and g the recovery rate. This model assumes a constant population size N, neglecting birth and death, so I + S = N. The objective of this section is to determine the evolution of the number of infected individuals, I(t), through time t, in order to show formally that identifiability will be a problem.

The number of susceptible agents can be written in terms of the total population size and the number of infected agents, specifically S = N - I. Thus only a single ODE need to be considered to calculate the rate of change in the number of infected agents

$$\frac{dI}{dt} = a(N - I) + b(N - I)I - gI.$$
(4.5)

To simplify the notation it is rescaled. This involves replacing I by the scaled variable x with rescaling parameter D,

$$I = Dx$$
,

and t is replaced by the scaled time τ with rescaling parameter T,

$$\tau = Tt.$$

The time rescaling can be interpreted in the following way: assuming $\tau = 1$ hour, and t = 1 minute, then the conversion factor from minutes to hours is $T = \frac{1}{60}$. The time derivative then becomes

$$\frac{d}{dt} = \frac{d\tau}{dt}\frac{d}{d\tau},$$
$$= T\frac{d}{d\tau}.$$

Substituting the new units into Eqn. (4.5) yields

$$TD\dot{x} = a(N - Dx) + b(N - Dx)Dx - gDx,$$
(4.6)

where the dot still refers to differentiation with respect to time. Dividing through by T and D gives

$$\dot{x} = \frac{a}{T} \left(\frac{N}{D} - x \right) + \frac{b}{T} \left(\frac{N}{D} - x \right) Dx - \frac{gx}{T}$$

which motivates choosing T = g to set the rate of recovery (from infected to susceptible) to 1, and D = N to make x the fraction of infected agents. Setting

 $\alpha = \frac{a}{g}$ and $\beta = \frac{bN}{g}$ results in the rescaled differential equation

$$\dot{x} = \alpha(1 - x) + \beta(1 - x)x - x.$$
(4.7)

This process began with three unknown parameters in Eqn. (4.5), rescaling has reduced the unknowns to just α and β .

Note that

$$\dot{x} = \alpha (1 - x) + \beta (1 - x)x - x = \alpha + (\beta - \alpha - 1)x - \beta x^{2}.$$
(4.8)

Writing the right-hand side of Eqn. 4.7 as a quadratic can help understand the dynamics and derive the steady-state equilibrium. In solving the quadratic for the roots, unstable and stable roots respectively, would describe the equilibria.

The equilibria can be found by solving

$$0 = \alpha + (\beta - \alpha - 1)x - \beta x^2,$$

or equivalently

$$0 = x^2 - \frac{\beta - \alpha - 1}{\beta}x - \frac{\alpha}{\beta},$$

which has solutions

$$x_{\pm} = \frac{1}{2} \left(\frac{\beta - \alpha - 1}{\beta} \pm \sqrt{\left(\frac{\beta - \alpha - 1}{\beta}\right)^2 + \frac{4\alpha}{\beta}} \right).$$
(4.9)

To determine whether the roots are real or complex conjugate roots, the numbers under the square root in Eqn. (4.9) should be considered. From this square root, observe that $\left(\frac{\beta-\alpha-1}{\beta}\right)^2$ is squared and so will always be positive and since α and β are both positive rates, $\frac{4\alpha}{\beta}$ is also positive. Thus everything under the square root will always be positive and so are real equilibria, with one positive root and one negative root.

Also, in this study of the ODE model, bifurcations are a possibility. Bifurcations occur when a small smooth change made to the parameter values changes the behaviour of the entire system (Blanchard, Devaney, and Hall 2006). In this case, if parameter values were changed so that the equilibria were to disappear, the parameter values would have to be negative. Therefore, though bifurcations can occur, they won't be considered and focus is placed on positive parameter values.

To learn the evolution of the number of infected through time, Eqn. (4.9) can be rewritten and then solved using the separation of variables. Then, the roots in Eqn. (4.9) can be used to factorise the right-hand-side of the ODE,

$$\dot{x} = -\beta(x - x_+)(x - x_-),$$

then separation of variables yields

$$\int \frac{dx}{(x-x_{+})(x-x_{-})} = \int -\beta d\tau.$$
(4.10)

Eqn. (4.10) can be solved with partial fractions, from which the following is found

$$\frac{1}{(x-x_{+})(x-x_{-})} = \frac{1}{(x-x_{+})(x_{+}-x_{-})} - \frac{1}{(x-x_{-})(x_{+}-x_{-})},$$

and substituting this into Eqn. 4.10 results in

$$\int \frac{1}{(x-x_{+})} - \frac{1}{(x-x_{-})} dx = -\beta(x_{+}-x_{-})\tau + \text{constant.}$$

Thus

$$\ln\left(\frac{x-x_{+}}{x-x_{-}}\right) = -\beta(x_{+}-x_{-})\tau + \text{constant},$$

and so

$$\frac{x - x_{+}}{x - x_{-}} = A \exp\left(-\beta (x_{+} - x_{-})\tau\right),\tag{4.11}$$

where A is a constant of integration.

Setting $x(0) = x_0$, the following is found

$$\frac{x_0 - x_+}{x_0 - x_-} = A.$$

Then, plugging the above into Eqn. (4.11) which gives

$$\frac{x - x_+}{x - x_-} = \frac{x_0 - x_+}{x_0 - x_-} \exp\left(-\beta(x_+ - x_-)\tau\right).$$

To return to solutions for I(t), the results from rescaling can be plugged in

$$x_{\pm} = \frac{I_{\pm}}{N},$$

where

$$I_{\pm} = I_{\pm} = \frac{1}{2b} \left(bN - a - g \pm \sqrt{(bN - a - g)^2 + 4abN} \right).$$
(4.12)

Consequently

$$\frac{I-I_{+}}{I-I_{-}} = \frac{I_{0}-I_{+}}{I_{0}-I_{-}} \exp\left(-\frac{b\mathcal{N}}{\not g}\frac{I_{+}-I_{-}}{\mathcal{N}}\not gt\right)$$
(4.13)

which can be rearranged to give

$$p = \frac{I_0 - I_+}{I_0 - I_-},$$
$$q = b(I_+ - I_-),$$

then

$$\frac{I - I_+}{I - I_-} = p \exp(-qt),$$
$$I - I_+ = p(I - I_-) \exp(-qt)$$
$$I - I_+ = p \exp(-qt)I - p \exp(-qt)I_-$$

$$I(t) = \frac{I_{+} - p \exp(-qt)I_{-}}{1 - p \exp(-qt)}.$$
(4.14)

From $I\pm$ (Eqn 4.9), the evolution of I(t) (Eqn 4.14) has been found. With these solutions, the Number of Panicked agents can be visualised, as done in previous sections with the case study ABM. Using the similar parameter values that were used to initialise the homogeneous configuration of the case study ABM, Table 4.11 summarises the values used to initialise the ODE. Figure 4.21 presents the evolution of I(t), otherwise known as the Number of Panicked Agents.

ODE Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	100	
Number of Agent Groups	1	
α	0.1	
β	0.386	
γ	0.2	

Table 4.11: ODE Model: Parameter Values

As anticipated, Figure 4.21 presents similar dynamics as seen in the homogeneous configuration of the case study ABM, over 100 iterations. The most perceivable difference is the absence of

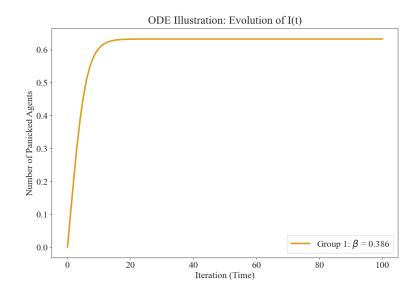


Figure 4.21: Number of Panicked Agents: Evolution of I(t) (Eqn 4.14)

stochasticity, formally presented in the peaks and troughs as seen in Figure 4.4. Having established the similarities between the homogeneous case study ABM and ODE model dynamics and findings will allow for parallels to be drawn in the investigation of parameter identification in Chapter 6.

In addition to the above, Table 4.12 presents the roots of the quadratic Eqn. (4.9), that were used to find the evolution of I(t).

I(m)	I(p)
-409.635	632.433

Table 4.12: Solutions for $I \pm (\text{Eqn 4.9})$

4.7 Summary - Modelling Contagion

The chapter began by first presenting the simple ABM based on the SISa model framework outlined in Chapter 3. The ABM was outlined using the overview design concepts and details (ODD) protocol outlined by Grimm, Berger, DeAngelis, et al. (2010) to describe the systems processes most appropriately. Section 4.3 presented the dynamics of the homogeneous configuration by fixing the Agent Parameters: α , β , γ and Number of Agent Groups, whilst varying the Model Parameters: Number of Agents, Number of Iterations and Model Instances. Then, heterogeneity was introduced by increasing the Number of Agent Groups. The dynamics of the output in the homogeneous and heterogeneous configurations were compared and found to be fundamentally similar. Section 4.4 investigated the impact of Agent Parameters on the output, whilst fixing the Model Parameters. Section 4.5 distinguished parameter values which were suitable based on the size of their effect on the output: in summary, the impact of α was most observable when small, whilst β and γ were most effective when bigger. Finally, Section 4.6 introduced an ODE model of emotional contagion that will be used in subsequent chapters to further investigate the impact of heterogeneity.

Chapter 5

Model Calibration

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5.1 Chapter Overview

Validation provides an assessment of how well the model approximates the real-world system and satisfies the research objectives; which in turn depends on parameter estimation and model calibration (Zhang, Li, and Zhang 2020). Model validation determines the robustness of statistical or computational experiment results and it serves as a basis for decision-making and future research (Berger, Manson, and Parker 2002).

Parameter estimation attempts to approximate the unknown parameters from empirical data, given some stochasticity. Estimated parameters discovered from the parameter estimation process fulfil a selection of conditions that distinguish them as true values. Effectively, parameter estimation presents the effects of a subset of parameter values within the model (Aster, Borchers, and Thurber 2019). Although the effects of the estimated parameters can be recognised and accepted as

significant, they may not be uniquely distinguishable from a wider subset of estimates. Model calibration is the process of distinguishing the estimates that reflect a particular known dataset (Tsai et al. 2021). When parameter estimates cannot be uniquely determined from the observed data, there exist one or more potential estimates that may produce predicted results similar to the observed data. This is known as the *parameter identification* problem which will be explored further in Chapter 6.

Even so, this is why model calibration is an essential process, as ideally, it determines a *unique* set of model parameters that provide a good description of the system behaviour (Judd and Judd 2011). Generally, calibration is an iterative process that fine-tunes the estimated parameters, holding its kind and structure constant. It effectively captures uncertainty so it can be understood but also quantified to help determine model reliability. Quantifying uncertainty, as with calibration and validation remains an ongoing challenge in agent-based modelling (Windrum, Fagiolo, and Moneta 2007; Crooks, Castle, and Batty 2008; Filatova et al. 2013; Heppenstall, Crooks, Malleson, et al. 2021). Uncertainty quantification is crucial to verifying model credibility when much has been invested in deterministic analyses and unwarranted assumptions (Smith 2013). This can be captured in calibration, as the process describes the inverse operation targeting optimal prediction and refers to the inference of best uncertain model estimates from experimental data (Hessling 2017).

Literature has defined two types of uncertainty quantification: forward uncertainty propagation and inverse uncertainty quantification. Forward uncertainty propagation investigates the impact of random inputs on the model outputs, this is commonly referred to as sensitivity analysis as seen in Chapter 4. On the other hand, inverse uncertainty quantification uses model outputs to determine sources of modelling uncertainty, through the process of parameter estimation or calibration (Arendt, Apley, and Chen 2012). This chapter will present inverse uncertainty quantification, mainly the model calibration process within the context of the case study ABM.

The calibration of ABMs is a challenging task. Due to the complexity of real systems in which ABMs are modelled, they typically contain a large number of parameters that need to be calibrated. And as the parameter space increases geometrically, this introduces a dimensionality problem (Lee

et al. 2015). High dimensionality, or increasing heterogeneity, requires increased computational capabilities when searching for significant parameter combinations, which can be computationally expensive for researchers (Zhang, Li, and Zhang 2020). One of the criticisms against ABMs is the lack of objective verification criteria, which affect replicability and scientific validation achieved through further study (Assenza, Delli Gatti, and Grazzini 2015; Caiani et al. 2016; Popoyan, Napoletano, and Roventini 2017). Consequently, there are a plethora of sources from which uncertainty can stem through the model. Some acknowledged sources include parameter uncertainty, model discrepancy, ensemble variance, and observation uncertainty (Kennedy and O'Hagan 2001).

Given this study's overarching aim, the calibration application differs from the common use in empirical ABMs. Calibration often involves the fine-tuning of estimates to observed or observational data, within this process, parameter uncertainty is captured. Parameter uncertainty can result from difficulties distinguishing which parameter values to use. Thus, calibration will be used as a detection tool to examine the parameter space to understand the impact heterogeneity may have on the case study model using synthetic data. To conduct this examination Approximate Bayesian Computation (ABC) calibration will be used. The following sections will briefly describe the method and present the results of the case-study model outlined in Chapter 4.

5.2 Approximate Bayesian Computation (ABC)

Bayesian statistics express probability as a degree of belief in the occurrence of an event (Gelman 2014), it considers old and new information through the systematic updating of beliefs (Forbes 2011). Bayes' theorem, which underpins all Bayesian statistical methods, suggests that given two events A and B, the probability of A occurring is conditional on event B having already occurred. This conditional probability is expressed mathematically as:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}.$$
(5.1)

Where, P(A|B) describes the probability of A occurring given B has already happened and P(B|A) is the probability of B given A has happened, P(A) and P(B) are the unconditional probabilities of A and B happening respectively. Principally, all the available information is used to infer the likely value of the given parameter.

Bayesian statistical methods are comprised of three components (Bayes 1763; Stigler 1986):

- 1. A Prior distribution, P(A), that describes all the knowledge and information available or *prior* beliefs regarding the occurrence of the event. Uncertainty is captured by the variance of the priors distribution; the larger the variance the more perceived uncertainty is assumed to exist.
- 2. *A Likelihood*, P(B|A), that poses the following question: Given the model parameters and available information, such as the mean and variance of the prior distribution, what is the probability of the event occurrence?
- 3. A Posterior distribution, P(A|B), is the combination of the prior distribution and likelihood function. It reflects the updated knowledge, balancing prior knowledge with the observed data.

Hence, Equation 5.1 can be simplified to Posterior \propto Likelihood \times Prior, where the posterior probability is proportional to the result of the prior probability and the likelihood function. When the likelihood is known, the posterior distribution can be easily derived directly and continuously

inferred as new data becomes available. However, in most cases, the likelihood function can be nearly impossible to derive, depending on the complexity of the problem. In these instances, Approximate Bayesian Computation (ABC) methods can be implemented to replace the likelihood function and determine an approximation for the posterior distribution based on samples. In ABMs, likelihood functions are often intractable due to model complexity; but more recently ABC has been proposed as an adequate substitute to achieve calibration (Turner and Van Zandt 2012; Grazzini, Richiardi, and Tsionas 2017).

ABC methods are algorithms used to estimate the posterior distributions of given parameters by sampling and simulating values from the prior repeatedly to produce synthetic datasets. The distance between the synthetic dataset and the observed data is calculated, and samples with comparatively smaller distances are accepted and form part of the posterior distribution. There are various ABC algorithms which have been applied in literature (Beaumont, Zhang, and Balding 2002; Beaumont 2010; Sottoriva and Tavaré 2010; Hartig et al. 2011; Martínez et al. 2011; May, Giladi, et al. 2013; Thiele, Kurth, and Grimm 2014; McCulloch et al. 2022; Zbair, Qaffou, and Hilal 2023), although the common ones are rejection sampling and sequential Monte Carlo.

5.2.1 ABC in Python: pyABC Package

The objective of this study is not the calibration process, but more to evaluate parameter space to conceive the impact of heterogeneity. The algorithm applied to the case-study ABM was the Approximate Bayesian Computation Sequential Monte Carlo (ABC-SMC) method, first developed by Del Moral, Doucet, and Jasra (2006) and Sisson, Fan, and Tanaka (2009); and made accessible through the open-source python toolbox pyABC package (Schälte et al. 2022).

The ABC-SMC algorithm filters samples of proposed values for a given parameter, the accepted values form the desired posterior distribution for the parameter. At each step of the algorithm, different combinations of parameter values are assigned weights proportional to their likelihood or posterior value. To avoid equal or close to zero weights, ABC-SMC includes a resampling step that adds new sets of values based on the weight distribution of accepted values (Grazzini, Richiardi, and Tsionas 2017).

To solve this parameter inference problem in the observation of the parameter space, as in to approximate model inputs from the model output, pyABC can be described as a backward parameter inference step. To operate, pyABC would require the following properties:

- A Model: pyABC accepts any model that produces a form of experimentally observed or synthetically generated data.
- A Distance Function: the specified measurements of the closeness between the observed and simulated data.
- **Parameter Priors:** probability distributions which represent uncertainty about the unknown parameters.
- Algorithm Stopping Functions: tolerance thresholds that must be satisfied will stop further sampling and terminate the algorithm.

Figure 5.1 summarised the pyABC process.

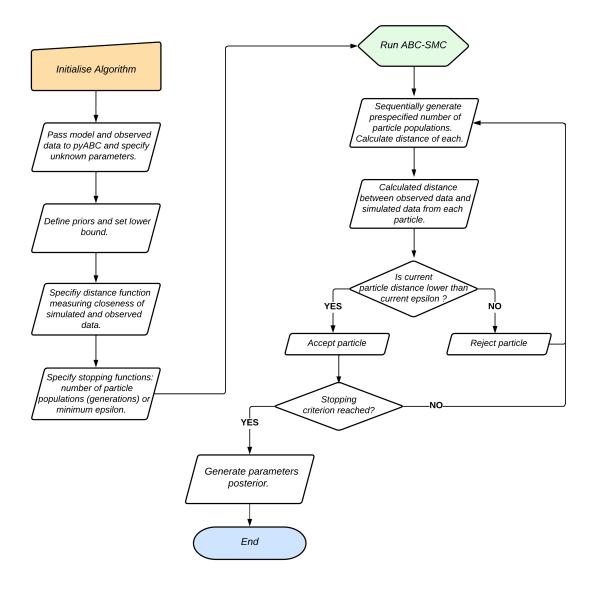


Figure 5.1: Flowchart summarising pyABC process.

5.2.2 Homogeneous Configuration

Table B.1 contains the input used to initialise the model and Figure B.1 presents the output or observed data, the Number of Infected. The CDF of the observed data, also pyABC¹ input, is illustrated in Figure 5.2.

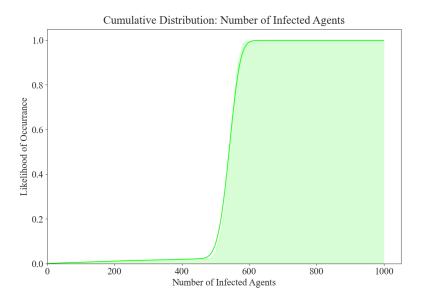


Figure 5.2: Cumulative Distribution of the Number of Infected

Three different observation formats were considered: the Number of Infected as a single value (i.e., the Total Number of Infected from a Single Iteration), a list (i.e., the full Number of Infected of a Single Iteration) or as a cumulative distribution function (CDF) of the Number of Infected. Following some initial experiments, the CDF produced the most accurate results; this is because the CDF accumulates probabilities for all possible values of the observed data and more appropriately captures dynamics that a single value or array could not. Figure 5.2 presents the CDF of the Number of Infected.

The distance between the observed and simulated data is calculated using the root mean square error (RMSE). Of the two stopping functions the Maximum Number of Populations was chosen over the use of Epsilon (ϵ) or both. As the aim was to minimise the distance between observed

¹The script for pyABC calibration can be found on Github, here.

and simulated data, the objective would be to achieve $\epsilon = 0$ which would be difficult to achieve; nevertheless, capturing how long (i.e., Maximum Number of Populations) it would take to achieve this was a more attainable experiment.

The Maximum Number of Populations denotes the number of generations by which the population is refined, each generation sequentially improves the approximation until the final population is reached. Selecting an appropriate population size is case-dependent, thus it is unfortunately difficult to give useful general guidelines (Del Moral, Doucet, and Jasra 2012). However, it is understood that too small of a population size yields large approximation errors, which hampers convergence, while too large population sizes result in an unnecessary computational burden (Klinger and Hasenauer 2017). This investigation will consider the Maximum Number of Populations typically used in pyABC examples as default, this number is 10 but will explore a further 2 generations to investigate whether the additional generations improved model performance. Therefore, the Maximum Number of Populations will be fixed at 12.

Additionally, each population sequentially generates particle populations of size 1000. And lastly, the mean for each parameter prior is assumed to be uniform over the intervals 0.0-0.1 and 0.0-1.0, for α and β , respectively (see, Figure 5.3). As α and β were rates of infection, a lower bound of 0.0 is specified to ensure posteriors were always non-negative.

pyABC ABC-SMC Algorithm Input		
Parameter	Value	
Data	CDF (Number of Infected)	
Distance Function	RMSE	
Max. No of Populations	12	
Population Size	1000	
Epsilon (ϵ)	Unspecified	
α	U(0.0, 0.1)	
β	\mathcal{U} (0.0, 1.0)	

Table 5.1: pyABC ABC-SMC Algorithm Input: Homogeneous Configuration

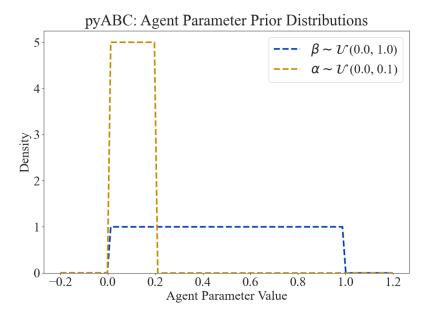


Figure 5.3: pyABC Priors: Alpha and Beta Parameters are Uniformly Distributed

To operate, pyABC required four properties: the model, a distance function, parameter priors and algorithm-stopping functions, which are outlined in Table 5.1.

Effectively, pyABC identifies which particle parameters are well-matching and which ones are not. The conditional probabilities are revised and updated until the select stopping criteria are satisfied; in this case, Max. No of Populations = 12.

Figure 5.4 presents the evolution of α and β from uniformly distributed priors to posterior distributions; where the final population (No. of Populations = 11) is assumed to be the most improved posterior, attributed with the smallest ϵ . To indicate the true values for reference, each figure is annotated with a blue-dashed line. As predicted, there seems some gradual convergence of the distributions so that they peak around the true values, with the width of the distribution capturing the uncertainty. The maximum a posteriori probability (MAP) estimate or the mode of the posterior distributions in each Population and credibility intervals are captured and presented in Table 5.2. As the final population (No. of Populations = 11) is the most improved, pyABC identifies 0.01595468 and 0.18851214 as the most common Bayesian point estimates for α and β , respectively.

pyABC then uses the information provided to produce conditional probabilities of the unknown parameters, α and β . The result, the posterior distributions, are visualised in Figure 5.4.

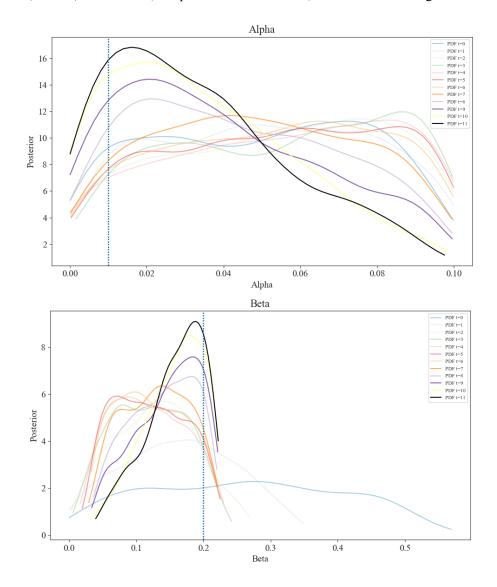


Figure 5.4: pyABC Posteriors: Conditional Probability of Alpha and Beta Parameters

5.2. APPROXIMATE BAYESIAN COMPUTATION (ABC)

Most interestingly, the true values of α and β , denoted by the blue-dashed line, are off-peak, this could potentially be attributed to the inherent stochasticity of the case study ABM. Essentially, given the observed data, these values could be substitute inputs used to initialise the case study ABM and reproduce dynamics that resemble the true CDF.

pyABC Algorithm Output: Posterior Modes				
Mode				
α	CI	eta	CI	
0.07139129	0.000155-0.099863	0.27874183	0.000211-0.568936	
0.0490366	0.000122-0.099990	0.17799358	0.000151-0.348723	
0.07540661	0.000108-0.099828	0.13861517	0.003125-0.268686	
0.08566693	0.001589-0.099680	0.07797279	0.005606-0.242005	
0.08360147	0.000003-0.099913	0.09069103	0.016513-0.230320	
0.08573803	0.000294-0.099979	0.06979561	0.019479-0.224940	
0.06521725	0.000034-0.099846	0.09823501	0.032885-0.221247	
0.04069004	0.000156-0.099465	0.13899384	0.029131-0.221391	
0.02032493	0.000016-0.099529	0.18239518	0.036208-0.219879	
0.02034568	0.000023-0.099606	0.18306601	0.0336880-0.221368	
0.02016144	0.000060-0.098556	0.17749642	0.037910-0.222768	
0.01595468	0.000026-0.097591	0.18851214	0.039572-0.222024	
	α 0.07139129 0.0490366 0.07540661 0.08566693 0.08360147 0.08573803 0.06521725 0.04069004 0.02032493 0.02016144	α CI 0.07139129 0.000155-0.099863 0.0490366 0.000122-0.099990 0.07540661 0.000108-0.099828 0.08566693 0.001589-0.099680 0.08360147 0.00003-0.099913 0.08573803 0.000294-0.099979 0.06521725 0.000034-0.099846 0.04069004 0.000156-0.099465 0.02032493 0.000023-0.099606 0.02016144 0.000060-0.098556	Λ <i>L M</i> α CI β 0.07139129 0.000155-0.099863 0.27874183 0.0490366 0.000122-0.099900 0.17799358 0.07540661 0.000108-0.099828 0.13861517 0.08566693 0.001589-0.099680 0.07797279 0.08360147 0.00003-0.099913 0.09069103 0.08573803 0.000294-0.099979 0.06979561 0.065521725 0.000034-0.099846 0.09823501 0.04069004 0.000156-0.099465 0.13899384 0.02032493 0.000023-0.099606 0.18239518 0.02034568 0.000023-0.099606 0.18306601 0.02016144 0.000060-0.098556 0.17749642	

Table 5.2: pyABC Posteriors: Posterior Mode of Alpha and Beta Parameters

Figure 5.5 visualises the credibility intervals around these posterior modes which show that the true values are within the 95% credibility interval and the maximum a posteriori probability (MAP) estimate (i.e., the posterior mode) seems to converge.

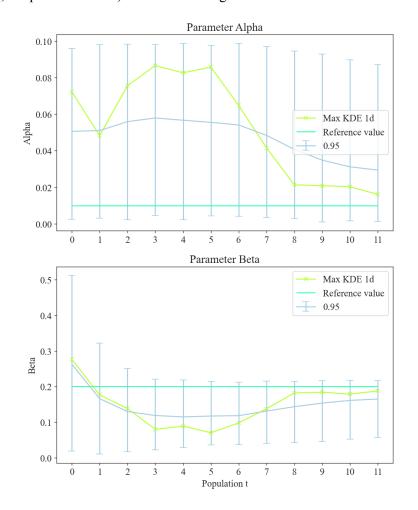


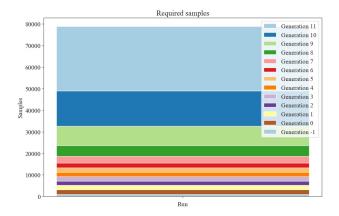
Figure 5.5: pyABC Posteriors: Credible Intervals for Alpha and Beta

Correspondingly, Figure 5.6 summarises the posterior estimation analysis, it considers the convergence and stability of each parameter by assessing posterior approximations at different generations and effective population sizes, across multiple runs. Figure 5.6a presents the *Required Samples* which captures the number of accepted samples required before particles are eventually rejected in each generation. Given the minimisation objective of pyABC, the initial generations are expected to have lower accepted samples which eventually improved through generations (or populations). This is demonstrated in this exercise, as the last generation, Generation 11, had the largest number of required samples and is considered the most improved posterior.

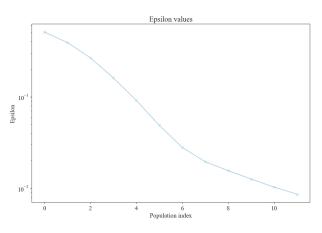
Figure 5.6b presents the *Epsilon Values* which denotes the decreasing acceptable threshold, ϵ , where Generation 11 achieves the lowest value. And lastly, Figure 5.6c presents the *Effective Sample Size* of each population and illustrates the most effective sample sizes through each generation. It suggests, that even though each particle considers the sample of 1000, by Generation 11, 1000 proves to be no more robust than a random sample of 600.

This exercise demonstrates model calibration using ABC to determine posterior distributions for α and β from a parameter space. pyABC provides significant results in the homogeneous configuration of the case study ABM this is proven by the success of parameter estimation and calibration. This begs to question whether the added complexity of heterogeneity could impact the quality of the results. This subsequent section considers this case by introducing heterogeneity, through additional β parameters.

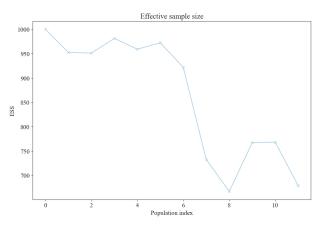
CHAPTER 5. MODEL CALIBRATION



(a) Posterior Estimation Analysis: Required Samples



(b) Posterior Estimation Analysis: Epsilon Values



(c) Posterior Estimation Analysis: Effective Sample Size

Figure 5.6: Homogeneous Config: pyABC Posterior Estimation Analysis

5.2.3 Heterogeneous Configuration

In this study, heterogeneity refers distinctively to agent granularity. As defined in previous chapters, agent granularity considers the coarseness of descriptive attributes and behaviours assigned to the agent component of ABMs. Though various approaches and methods exist to introduce heterogeneity, in this exercise, heterogeneity is introduced by increasing the Number of Agent Groups and assigning each group a unique rate of infection, β .

The simple sensitivity analysis conducted in Section 4.4, proposes assigning β values to Agent Groups which produce dynamic outputs that are distinguishable. Thus, $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$ were assigned the values 0.2 and 0.6, respectively. Figure B.2 illustrates the Number of Infected for $\beta_{\text{Group 1}}$, $\beta_{\text{Group 2}}$ which produces the expected dynamics: the group with the highest β presents with a larger proportion of infected agents. The Total Number of Infected will be used as model output, to ensure consistent results against the homogeneous configurations. Table B.2 contains input used to initialise the ABM and can also be found in Appendix B.

Table 5.3 contains the input used to initialise pyABC and Figure 5.7 visualises the CDF of the Total Number of Infected.

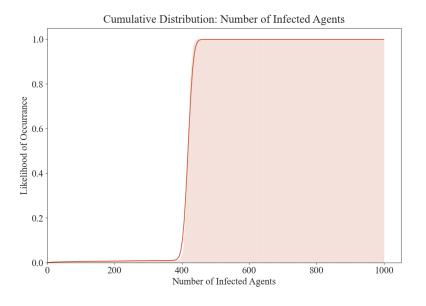


Figure 5.7: Heterogeneous Config: Cumulative Distribution of the Total Number of Infected

pyABC² properties are fixed, sharing the same values as in the homogeneous configuration.³ Figure 5.8 visualises the priors.

pyABC ABC-SMC Algorithm Input		
Parameter	Value	
Data	CDF (Number of Infected)	
Distance Function	RMSE	
Max. No of Populations	12	
Population Size	1000	
Epsilon (ϵ)	Unspecified	
α	$\mathcal{U}\left(0.0,0.1 ight)$	
$\beta_{\text{Group 1}}$	${\cal U}$ (0.0, 1.0)	
$eta_{ ext{Group 2}}$	U(0.0, 1.0)	

Table 5.3: pyABC ABC-SMC Algorithm Input: Heterogeneous Configuration

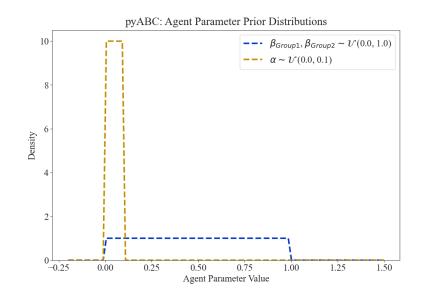


Figure 5.8: pyABC Priors: Alpha and Beta Parameters are Uniformly Distributed

²The script for pyABC calibration can be found on Github, here.

³A further experiment constraining the prior distributions were performed any better than when the priors were constrained, see Appendix B.3.

Figure 5.9 depicts the evolution of α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$. Where the true parameter values are indicated by the vertical blue-dashed lines, α and $\beta_{\text{Group 1}}$ posteriors perform adequately in their movement and convergence towards the truth, with some uncertainty. However, pyABC seemingly presents with some difficulties when estimating $\beta_{\text{Group 2}}$ and the difference is noteworthy. Table 5.4 presents the posterior modes and credible intervals, from here the most improved generation (No. of Populations = 11), produced 0.01850757, 0.24232129 and 0.23383305 as estimate values for α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$, respectively. Figure 5.9 illustrates the credible intervals for each posterior. Although the true values and posterior modes are within the 95% credibility interval, MAP fails to converge around the true $\beta_{\text{Group 2}}$ value.

To consider pyABC performance, Figure 5.11 presents the posterior estimation analysis. As with the homogeneous configuration, Figure 5.11a presents the *Required Samples* which captures the number of accepted samples required before particles are eventually rejected in each generation. As generations progress, pyABC accepts more samples and as one might expect, Generation 11 has the largest number of accepted samples and thus is considered the most improved posterior. Similarly, the true values of α and $\beta_{\text{Group 1}}$ are off-peak but still within proximity of the true values. As previously suggested in the homogeneous Configuration, this off-peak could be attributed to the inherent stochasticity. However, $\beta_{\text{Group 2}}$ has been gravely underestimated by pyABC. This distance may be more indicative of poor parameter estimation.

Similarly, Figure 5.11b presents the *Epsilon Values* which exhibits a decreasing acceptable threshold, ϵ , where Generation 11 achieves the lowest value. And lastly, Figure 5.11c presents the *Effective Sample Size* illustrating the most effective sample size through each generation. Though decreasing through generations, it suggests that by Generation 11, 1000 particles prove to be no more robust than a random sample of 700.

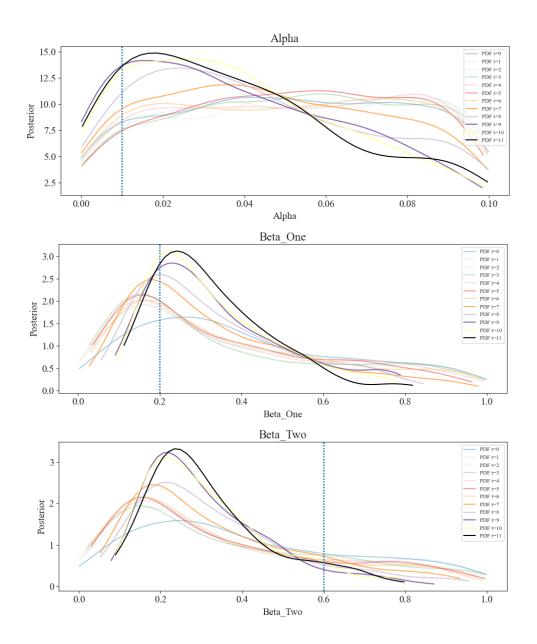


Figure 5.9: pyABC Posteriors: Conditional Probability of Alpha and Beta Parameters

pyABC Algorithm Output: Posterior Modes						
Na of Domilations	Mode					
No. of Populations	α	CI	$eta_{ ext{Group 1}}$	CI	$\beta_{ m Group\ 2}$	CI
0	0.04283452	0.000014-0.099929	0.26767779	0.003541-0.999132	0.24527902	0.000716-0.999349
1	0.08366699	0.000213-0.099951	0.16416398	0.001548-0.997573	0.16355329	0.000814-0.997592
2	0.04898953	0.000025-0.099995	0.14920186	0.008112-0.995739	0.16330774	0.000282-0.998817
3	0.05940693	0.000672-0.099914	0.14652457	0.028646-0.991324	0.15906474	0.019704-0.995232
4	0.0814778	0.000053-0.099798	0.16532287	0.027080-0.994782	0.15327569	0.0152142-0.981645
5	0.05839731	0.000088-0.098610	0.15024702	0.036793-0.963336	0.14823908	0.030032-0.995388
6	0.07337076	0.000540-0.099671	0.16676716	0.030604-0.983748	0.16708658	0.030072-0.989175
7	0.03661728	0.000046-0.099601	0.18288615	0.027461-0.979439	0.17787507	0.051866-0.933927
8	0.02457723	0.000158-0.099869	0.20158132	0.057027-0.844045	0.21761184	0.051663-0.955160
9	0.01609001	0.000039-0.098353	0.23377126	0.091506-0.788605	0.20786238	0.078748-0.869573
10	0.02655735	0.000168-0.099635	0.21832509	0.092031-0.779631	0.2167801	0.087887-0.789639
11	0.01850757	0.000245-0.099676	0.24232129	0.112738-0.818246	0.23383305	0.089382-0.797193

Table 5.4: pyABC Output: Posterior Mode of α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$

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As with the previous exercise, pyABC determines approximate posterior distributions for the unknown parameter values α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$. Although the algorithm succeeds in determining multiple β values from uniform priors, it does not succeed in uniquely identifying all of them. Further, it has been shown that adjusting prior knowledge (i.e., constraining prior distributions of α and β to smaller intervals in both model configurations) only slightly improves pyABC performance (see Appendix B.3).

pyABC and the wider ABC framework provide a straightforward way to investigate the goodness of fit of the model, particularly when likelihood functions are unavailable or intractable, as in ABMs (Rogers-Smith, Pesonen, and Kaski 2018). Generally, the likelihood function would indicate the extent to which parameter values are congruent to the observed data. Approximate likelihoods can also achieve this, where a flat approximate likelihood surface would indicate issues with the distance function struggling to measure the differences between the observed and simulated data accurately. This is known as a parameter identification problem, where there exist several other parameter values that could produce data similar to the observed, true data (Lintusaari et al. 2016). This problem occurs when the model fails to appropriately capture the dynamics through the model inputs. It could be the result of *practical identification* issues, which relate to the data failing to provide sufficient information to identify the model parameters; or, a *structural identification* issue, which relates directly to inadequate model structures that prevent the effective capturing of information to identify the model parameters. Parameter identification will be investigated further in Chapter 6.

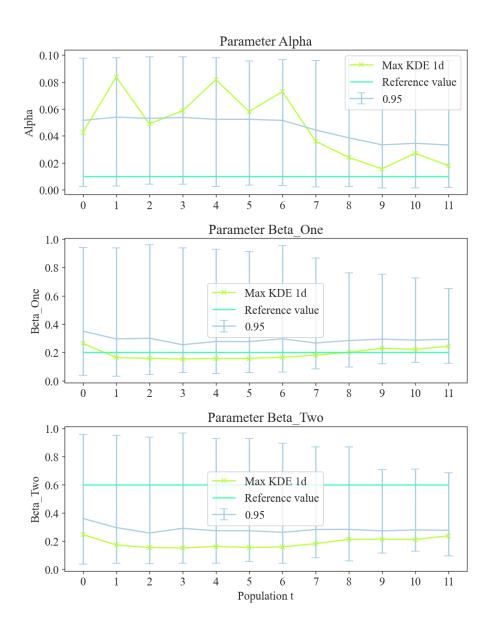
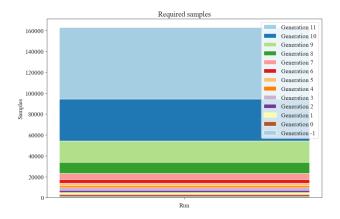


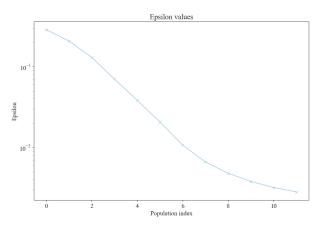
Figure 5.10: pyABC Posteriors: Credible Intervals for Alpha and Beta

5.2. APPROXIMATE BAYESIAN COMPUTATION (ABC)

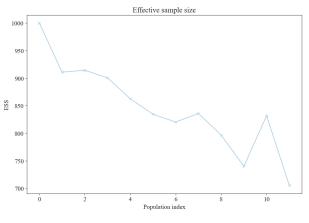
CHAPTER 5. MODEL CALIBRATION



(a) Posterior Estimation Analysis: Required Samples



(b) Posterior Estimation Analysis: Epsilon Values



(c) Posterior Estimation Analysis: Effective Sample Size

Figure 5.11: Heterogeneous Config: pyABC Posterior Estimation Analysis

5.3 Summary - Model Calibration

In this chapter, a series of calibration exercises were undertaken to explore the parameter space of the case study ABM. The purpose of this is to lay the groundwork for the investigation into the impact of heterogeneity as the result of a parameter identification problem in Chapter 6. Section 5.2 presents a series of exercises using pyABC on the case study model. This section demonstrates ABC methods as a robust tool, able to deliver accurate results and capture uncertainty. The accuracy is observed in the defined peaks which characterise the α and β posterior distributions. In light of the chapter objective, pyABC stand as an excellent tool for ABM calibration; but it does force researchers to consider their robustness when attempting to detect parameter identification.

Chapter 6

Impact of Heterogeneity: Parameter Identification

Contents

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6.2	Parameter Identification
6.3	Identification Analysis of Agent-Based Models
6.4	The Implications of Unresolved Structural Identification Issues 170
6.5	Summary - Parameter Identification

6.1 Chapter Overview

Heterogeneity refers to the individual features and attributes that form observable differences in human populations; within the scope of ABMs however, it relates to the concept of agent granularity as defined in Chapter 2. Agent granularity refers to the coarseness of the descriptive attributes and behaviours assigned in the agent component of ABMs (Gao, Song, and Wang 2013). This study assumes the more detailed or granular the agent attributes the more heterogeneous the agent population; the coarser the agent attributes the less heterogeneous the population. To assume

uniformity in agent granularity would be to define agent attributes in a single dimension or homogeneously. Whereas, assuming variability would define agent attributes multi-dimensionally or heterogeneously.

Modelling heterogeneously is the main advantage of ABMs, but due to their increasingly complex nature, it can make calibration a computationally challenging task. An often overlooked part of calibration, particularly with highly dimensional models, is the identification of parameters. Identification or identifiability issues refer to the presence of multiple plausible or 'optimal' model inputs that fit observed output reasonably well. This would have large implications for the application of the model and findings, as failure to identify parameters means the true model dynamics cannot be understood fully. Therefore, this thesis proposes *parameter identification* as the impact of heterogeneous modelling in ABMs. As heterogeneity refers to the number of parameters used to describe agents, where there is an increasing number of parameters this may introduce identification issues.

The previous chapters presented a simple toy model ABM as a tool to illustrate the concepts of homogeneity and heterogeneity; furthermore, sensitivity analysis and a series of calibration exercises were undertaken to explore the model dynamics and the parameter space. Briefly, sensitivity analysis and calibration are used as tools to capture model uncertainty, hence a degree of confidence can be assumed in model outputs. However, the various methods and approaches which exist for model calibration and analysis, either explicitly or implicitly acknowledge parameter identification. Therefore, parameter identification analysis cannot be separated from the model calibration process, and in fact, should be considered most pertinent to the calibration and model development cycle (Grimm and Railsback 2005).

This chapter will begin by presenting the concept of parameter identification and the standard analytical approaches to remedying the issue. Followed by an illustration of parameter identification issues using the ODE model and the case study ABM from Chapter 4. This study will then conclude by considering the implications of unresolved parameter identification issues in ABMs.

6.2 Parameter Identification

Chapter 2 presented the distinct forms of heterogeneity and advantages in ABM research. As already proposed, heterogeneity plays a central role in the appeal of ABMs and their widespread application; because of this, it is important to consider the possible impact of choosing to model heterogeneously.

The outcome of increasing agent granularity can be likened to the concept of *overfitting* seen in the evaluation of traditional statistical models. Overfitting arises from the structure of the machine-learning task; it occurs from the overtraining of a statistical algorithm to data which increases the risk of fitting noise, rather than finding general predictive rules (Dietterich 1995). Models which overfit are characterised by too many model terms for the number of observations. And the more "free" parameters in the model than the number of data points used to calibrate it, there exists an infinite number of observable equivalent parameterizations. This is known as the parameter identification issue (Brown, Hill, et al. 2004; Lipniacki et al. 2004; Achard and De Schutter 2006). Parameter identification is relevant to ABMs. Most ABMs are complicated as they contain a large number of parameters and structural assumptions (Sun et al. 2016). With limited knowledge of the processes and mathematical intractability, paired with limited empirical data to compare model output (Augusiak, Van Den Brink, and Grimm 2014; Ligmann-Zielinska et al. 2014); this gives rise to a mismatch between model and data dimensionality and multiple structures that generate outputs inconsistent with the data.

Furthermore, assessing model fit is a review of elements that constitute a useful model. A useful model is comprised of three components: firstly, it captures the main effects in the data with reasonable accuracy. Secondly, they produce hypotheses that can be tested experimentally. Thirdly, the model should gather insights about the target system. If a model satisfies the first and second components, it can be considered a good model. In fully parametric models, these components can be measured through the observation of information criterion which assesses the quality of a statistical model. However, due to stochasticity, feedback loops, and the non-analytical (i.e., no fixed structural form) nature of ABMs, the construction of the initial model is based on current knowledge or expertise. At this stage, the model cannot explain the data and therefore is consid-

ered a bad model. Based on trial and error, one increases model complexity until the data can be fitted which is a common approach. It is not hard to see how this approach can easily lead to the over-parameterization of the model to data. The model parameters and predictions are not well determined, and it thus remains a bad model.

Polhill and Salt (2017) demonstrate that the traditional measure of model goodness in measures of fit-to-data is not enough to determine how 'good' an ABM is. They propose that in addition to fit-to-data measures, the ABM's ontological structure should also be assessed. In computer science, ontology refers to a specification of a conceptualization of a given domain (Gruber 1993). Concerning ABMs, ontology refers generally to the development of a formal methodology which establishes common vocabulary used to define the concepts and relationships between those concepts of the system. As well as the reasoning about the objects, behaviours, and knowledge that comprise the system (Christley, Xiang, and Madey 2004). The most prevalent ontology language is the Web Ontology Language (OWL) (Horrocks, Patel-Schneider, and Van Harmelen 2003; Grau et al. 2008). The application of OWL to agent-based modelling has been discussed by several authors (Gotts and Polhill 2009; Pierre Livet 2010).

Polhill and Salt (2017) went on to compare various metrics and measures of validation, including vector norms, sum of squared and root mean squared errors stochastic methods such as likelihood, Akaike Information Criterion and Bayes Information Criterion. They concluded that there were clear advantages and disadvantages to each method, regardless of the results. Likewise, Brewer, Butler, and Cooksley (2016) previously demonstrated some controversy around determining which validation measures prediction ability could be the 'best'.

Notwithstanding, the general approach to improving the quality of a bad model involves the integration of additional data whilst simultaneously reducing model complexity until there is a balance between available data and model parameters. This process is iterative and can be laborious as it can be a computationally intensive task, and where data is unavailable may not even be possible. Parameter identification analysis has been linked to the improvement of bad models to good models; as the objective of this process is to create good models that can describe the data and have well-determined parameters and predictions.

Parameter identification has two types: structural and practical identification (Godfrey and DiStefano 1985). A structural identification problem would arise *a-priori* on the structural properties of a model which depends only on system dynamics, the observation and the stimuli functions (DiStefano and Cobelli 1980; Walter and Pronzato 1997). A practical identification problem arises *a-posteriori* and relates to the numerical values of parameters determined from data (DiStefano and Mori 1977). The objective of this section is to present a brief summary of traditional approaches used to conduct analysis.

6.2.1 Practical Identification

The task of defining practical identification has been a challenging one. What is well understood amongst researchers, is the need to create models that adequately describe the data and have well-determined parameters to ensure robust predictions (Brown, Hill, et al. 2004; Lipniacki et al. 2004; Achard and De Schutter 2006). Identification literature describes the concept of practical identification rather broadly; generally across disciplines, it refers to a powerful, yet under-utilised tool able to support model-based analysis (Raue, Kreutz, Maiwald, et al. 2009; Hines, Middendorf, and Aldrich 2014; Saccomani and Thomaseth 2018; Wieland et al. 2021). Practical identification issues are variations in parameter estimates that arise as the result of experimental conditions and model structure issues¹. Conducting practical identification analyses provides useful quantification of parameter uncertainty (Lam, Docherty, and Murray 2022). In essence, practical identification would evaluate the size of measurement errors from parameter estimates and determine whether they fall within practically *'acceptable'* bounds (Vajda, Rabitz, et al. 1989). Consequently, a precise definition for this phenomenon is difficult to construct, as what is considered acceptable bounds will be distinctive across research and disciplines.

Based on identification literature, practical identification reaches beyond the assessment of model fit, as does parameter estimation, calibration and validation. It specifically considers the uniqueness of parameter fits in the presence of experimental considerations. In response to this gap in research, a field of study that explores the interconnections between optimal experimental design

¹Practical identification is also referred to as deterministic, numerical, or a-posteriori identifiability

and parameter estimation has increased in recent times (Balsa-Canto, Banga, and Alonso 2008; White et al. 2016; Krausch et al. 2019). An optimal experimental design, also refers to experimental infrastructure, optimises the quality of information obtained through model inputs, sampling times, initial conditions, and experiment duration (Pronzato 2008). Thus the overlap between practical identification analysis and optimal experimental design methods which this section will briefly present.

Sensitivity analysis is a standard tool used to capture uncertainty present in model outputs that are directly generated by uncertainty in the model input and parameterisation (Saltelli et al. 2008). From the sensitivity analysis, sensitivity matrices are created to rank the influence of parameters on model output, which in turn serves as an indication of unidentifiability (Gábor, Villaverde, and Banga 2017). Practical non-identification (or unidentifiability) in sensitivity analysis presents through parameters that would have no influence on model output. On the other hand, in cases where combinations of model inputs exhibit substantial yet similar model outputs, sensitivity analysis processes may incorrectly infer the practical identification from the observed sensitivity; though what this may indicate is the indistinguishable effects between model inputs, suggesting their influential effects could be compensated by equivalent changes to the other (Docherty et al. 2011; Joubert, Stigter, and Molenaar 2018).

The *Fisher information matrix* (FIM) measures the amount of information about parameters provided by experimental data (Fisher 1997) and is often used in experimental design to assess and optimise the design for maximizing the expected accuracy of parameter estimates (Kreutz and Timmer 2009). Fisher information is defined as the variance in the expected value of the observed information; if the function is characterised by a clear peak in the data the easier it is to indicate the 'correct' value of the model input from the model output. For multiple model inputs, fisher information takes the form of a matrix, describing the covariance between each pair of parameters.

Along with sensitivity analysis, FIM can be used to investigate practical identification. It can be expressed with the normalised sensitivity matrix and a measurement noise covariance matrix. FIM and the normalised sensitivity matrix are analysed through eigen-decomposition to determine whether the system may have identifiability issues. The eigenvalues and eigenvectors of FIM indicate the principal components and the directions of the variances (Yang, Langley, and Andrade 2022); a 'small' eigenvalue would indicate ill-conditioning of the matrix, due to there being an under-constrained parameter direction (Chis et al. 2016). Eigenvalues were also used to measure the 'sloppiness' or 'stiffness' of parameter estimates (Waterfall 2006; Gutenkunst, Casey, et al. 2007; Gutenkunst, Waterfall, et al. 2007; Transtrum, Machta, and Sethna 2010a,b; Transtrum, Machta, Brown, et al. 2015; Mannakee et al. 2016). Sloppy models are characterised by estimates that could vary massively without significantly influencing the model output. Whereas, stiff models produce parameter estimates which could be determined with great certainty (Raman, Anderson, and Papachristodoulou 2017). In this case, a 'large' eigenvalue would indicate a sloppy model. Although the concepts of practical identification and sloppiness have been likened, sloppiness may not imply the presence of non-identification and to achieve precise parameter estimation optimising practical identification would take priority over reducing model sloppiness (Chis et al. 2016). Nonetheless, considering multiple experimental protocols that enable changes in eigenvector from the concepts of sloppiness could be applied to identification problems (White et al. 2016). The types of experimental protocols that could impact eigenvectors include sampling times, varying inputs, and changing initial conditions (Gottu Mukkula and Paulen 2017). While sensitivity-based approaches to practical identification have low computational costs, the perturbations observed in sensitivity analysis have been questioned for even the simplest nonlinear models (Joshi, Seidel-Morgenstern, and Kremling 2006). It implies when measurement uncertainty is discrete, local sensitivity characteristics typically give poor approximations to uncertainty in parameter estimates.

Moreover, some Bayesian sampling approaches utilise *Monte Carlo* (MC) methods (Metropolis and Ulam 1949), and have been employed to assess the practical identification of parameter estimates (Siekmann, Sneyd, and Crampin 2012; Zuo et al. 2019). MC repeatedly simulates measurement noise on a dataset and can conduct backward parameter inference (or the inverse problem) on the noisy data to produce parameter estimates. This process is repeated many times to aggregate a set of parameter estimates. The following procedure using MC sampling was proposed (Miao et al. 2011): (1) identify the nominal parameter vector for study; (2) simulate the model with the parameter vector and obtain its measurements; (3) generate N sets of simulated data from the measurements with a given measurement error level; (4) fit the model to each of the N simulated datasets to obtain parameter estimates in the parameter vector; (5) calculate the average relative estimation error (ARE) for the parameter estimate.

The steps outlined above can be repeated for multiple noise levels to understand the relationship between practical identification and measurement noise. The ARE values indicate the identification of the parameter estimate; for example, if ARE produces a significantly higher noise value than the expected value, this implies practical non-identification. Naturally, what is declared as 'acceptable' or 'high' values would be distinct across various model-based analyses, thus there are no ARE thresholds to follow as guidance. This provides researchers with total decision-making power to determine practical identification based on the model context and their expertise. Yet, there are some limitations to ARE. ARE assumes the parameter estimates are centred around the parameter vector and do not indicate relationships behind parameters, which sensitivity-based analysis approaches accomplish. To overcome this problem, some studies have calculated pairwise correlations from the parameter estimates, even if they can only reveal linear relationships (Pironet et al. 2019; Lizarralde-Bejarano et al. 2020).

Another approach to conducting practical identification analyses is in the observation of parameter estimate *confidence intervals* (Busch et al. 2015; David and Ricard 2019; Duchesne et al. 2019; Zhou et al. 2020; Johnson et al. 2021). Confidence intervals are derived using FIM; where large individual and joint confidence regions were indicative of practical non-identification. Some studies proposed the large limits were linked to there being too many parameters to be estimated from the available measurements (Nihtilä and Virkkunen 1977; Holmberg 1982). Similarly, Lam, Docherty, and Murray (2022) constructed *sensitivity-based* 95% *confidence intervals* using FIM and compared results to the MC sampling approach to assessing practical identification in a linear toy model. They found that both methods produced similar results: where, 95.1 and 96.0% of the MC samples fell within the confidence intervals for the high and low noise levels, respectively. Despite these results, they proved the MC sampling approach to be more advantageous in cases where non-linearity is present (Krausch et al. 2019). Non-linearity is common in real-world models and FIM has the potential to misrepresent confidence intervals, therefore MC simulations are considered more appropriate to ensure parameter variances are quantified effectively.

Furthermore, the *profile likelihood* approach to assessing parameter estimates for practical identification has grown in popularity in recent times but has widespread use in system biology studies where it first emerged (Hug et al. 2013; Eisenberg and Hayashi 2014; Baker et al. 2015). The method generates 'profiles' of parameters by fixing a single parameter and fitting the remaining parameters to the data. The likelihood corresponding to each parameter value forms the likelihood profile across parameter space. This method can detect both structural and practical nonidentification in parameter estimates. Most practical identification studies use likelihood-based approaches, rather than asymptotic confidence intervals. Asymptotic confidence intervals, as seen above, use quadratic approximations of model residual error in close proximity to the estimated parameter values to extrapolate to a maximum estimated likelihood, whereas, likelihood-based confidence intervals are represented as borders of the neighbourhood of parameters around parameter estimates within a confidence region. Unlike asymptotic confidence intervals, likelihood-based confidence intervals are able to capture asymmetric parameter profiles and are considered superior when samples are finite (Neale and Miller 1997).

The likelihood approach iteratively profiles individual parameters to determine whether a parameter is unbounded in one direction. If so, then practical non-identification exists. As parameter profiles are created independently, the method can be parallelized for bigger models and larger datasets. Further, the profile likelihoods can be visually inspected over several model trajectories and indicate where additional measurements may capture more information (Raue, Becker, et al. 2010). What is most apparent from this short review, is the profile likelihood and MC approaches require robust optimisation methods to properly assess identification. The likelihood calculations re-optimise non-fixed parameters across regions where the likelihood may be flat or near-flat, evidence of practical non-identification. Failing to determine the global minima across the profile will result in an erratic profile, which can indicate possible optimisation failure or unusual local minima characteristics. A recent method extends the method to 2D profile likelihoods which can explore pairwise parameter interdependence, though it brings a significant increase in computational time (Brastein et al. 2019).

Though essential, the practical identification of ABMs will not be the focus of this study. This

study will consider identification issues which arise more specifically from the fundamental structure of ABMs and less so from the experimental designs and the description of data. This type of identification is referred to as structural identification, this concept will be presented and elaborated on in the following section.

6.2.2 Structural Identification

The definition of structural identification, in contrast to practical, has been more refined in parameter identification literature (Anstett-Collin, Denis-Vidal, and Millérioux 2020). Also referred to as theoretical or a-priori identification, structural identification investigates whether model inputs could be uniquely determined from any given model output (Bellman and Åström 1970; Cobelli and DiStefano 1980; Ljung and Glad 1994; Saccomani 2013). This type of issue often arises from the model and measurement (input–output) structure and is unrelated to model stimuli or experimental designs, thus cannot be resolved numerically (Massonis, Banga, and Villaverde 2021). Although overlooked due to the challenging nature of the problem, structural identification analysis is fundamental to guarantee unique parameterization exists regardless of the numerical estimation procedure implemented (Thomas, Chappell, et al. 1989; Pia Saccomani, Audoly, and D'Angiò 2003; Xia and Moog 2003; Verdiere et al. 2005; Raue, Karlsson, et al. 2014; Saccomani and Thomaseth 2016; Varghese, Narasimhan, and Bhatt 2018).

When parameters cannot be structurally identified, this suggests that changing the parameter does not affect the model's trajectory or output as its change could be compensated by altering other parameters (Wieland et al. 2021). There exists some distinction within structural identification globally and locally: where structural global identification refers to the distinguishing of all unknown parameters within a parameterised state space and structural local identification restricts the parameter space to a neighbourhood (Chappell, Godfrey, and Vajda 1990; Saccomani, Audoly, et al. 1997; Karlsson, Anguelova, and Jirstrand 2012; DiStefano 2015; Stigter and Molenaar 2015; Stigter, Beck, and Molenaar 2017). That said, it is possible for some parameters to be locally identifiable, but not globally. Structural identification analysis is partly comprised of methodologies that assist in a-priori model adaptation, as some analysis can be performed before evaluating model

fit. But in most cases, identification issues can only be remedied by reformulating² the model informed by model fit information. The relationship between practical and structural identification is most interesting; in that achieving structural identification would not imply the practical identification of model parameters. This would arise if there was an insufficient amount of data or data of poor quality and can be demonstrated through confidence intervals which are infinite (Saccomani and Thomaseth 2018).

As with practical identification and optimal experiments design, structural identification analysis has been linked to observability analysis. This section will briefly outline some approaches to conducting structural identification analyses, which involve the verification of the systems structure. The earliest technique employed the transfer function from system and control theory, specifically the input-output system map, for linear models but with a *Laplace transform*. Bellman and Åström (1970) proposed: as a systems input-output relation could be given by its impulse response, then structural identification could be achieved from impulse response measurements. Laplace transformation has an extensive history of successful applications and is still utilised in present times (Skinner et al. 1959; Distefano et al. 1975; Cobelli and DiStefano 1980; Godfrey 1986; Ovchinnikov, Pogudin, and Thompson 2019).

Another proposed method for analysing the structural identification in linear dynamic models is *generating power series expansion*. The generating power series expansion methods identify model symmetries using Lie algebra (Pohjanpalo 1978; Walter and Lecourtier 1982; Ligon et al. 2018). Methods based on Lie group theory propose symmetries in the system can be indicative of structural non-identification (Yates, Evans, and Chappell 2009; Merkt, Timmer, and Kaschek 2015; Villaverde et al. 2019; Massonis and Villaverde 2020). Essentially, the parameters which are observable are expanded in a series where the coefficients are the output functions and their successive Lie derivatives, with respect to time and inputs. Structural identification is achieved when the exhaustive summary coefficients and Lie derivatives are unique. However, the minimum number of required Lie derivatives to reach uniqueness is unknown and likely dependent on the model.

²In this case, model reformulation would involve reducing the number of states and parameters and fixing parameter values (Bandara et al. 2009). Whereas to solve practical non-identification this may involve considering the experimental constraints and designing sufficiently rich experiments (Balsa-Canto, Banga, and Alonso 2008)

The *taylor series* approach is based on a similar assumption: observations and their derivatives with respect to time should be unique. Therefore, observables can be represented by Taylor series expansion and its uniqueness would guarantee the structural identification of the system.

Further, the *similarity transformation* approach was derived from the local state isomorphism theorem (Walter and Lecourtier 1981; Vajda, Godfrey, and Rabitz 1989). Some pre-conditions to applying this method are controllability and observability³ and once fulfilled the model is locally reduced. Also, it's assumed that all bounded and measurable functions are available for stimulus. From here, the objective is to identify state variable transformations that leave the stimuli-observables map and the structure of the system unchanged. The local state isomorphism establishes a set of first-order linear in-homogeneous partial differential equations that are then used to construct the functional form of such transformations. However, the solution of the partial differential equations can be complex, and testing for controllability and observability conditions is difficult for non-linear systems. Although an alternative method was proposed that would capture direct relations of the components of the isomorphism, the process of assessing the observability condition remains challenging and the solving of the differential equations complex (Vajda and Rabitz 1989; Denis-Vidal and Joly-Blanchard 1996; Peeters and Hanzon 2005).

Moreover, the *differential algebra* method replaces the stimuli-observables behaviour of the system with polynomial or rational mapping (Ljung and Glad 1994). Differential state variables which are non-observable are removed to derive direct relationships between inputs, outputs and parameters. These relations are derived using Ollivier's method (Ollivier 1990). These relationships are collated into an exhaustive summary that can be obtained and solved using rigorous algebraic methods, such as the Buchberger algorithm (Buchberger 1976). The differential algebra approach utilises a variety of strategies which has been proposed for models described linearly and non-linearly, with or without information on the initial conditions. Naturally, the method assumes the model can be expressed in terms of polynomials or rational functions and controllability (Bellu et al. 2007). The exhaustive summary is considered an observable representation of the model,

³When controllability is assumed, the model can be used to illustrate or demonstrate any purpose, as the given dynamic system is controllable; Observability assumes the modeller has a full understanding of internal intricacies of model dynamics (Kalman 1960).

derived from differential polynomials and ranking processes. Structural identifiability is assessed by first normalising the differential polynomials, then checking the injectivity of the exhaustive summary (Margaria et al. 2001). This method provides precise information about parameter identification, but it comes with great computational requirements which only increase with model complexity.

The approaches outlined above can only be applied to rather low-dimensional systems, due to their computational and algebraic complexity. Most recently, there have been developments focusing on improving the computational efficiency of the algorithms, particularly for non-linear and increasingly complex models.

Developments on local sensitivity calculations and processes have been proposed, for example, the introduction of a comprehensive process which proposed to resolve structural non-identification by *reparameterization* of the model (Joubert, Stigter, and Molenaar 2020). The underlying concept of reparameterization assumed that the unidentified parameters could be categorised into different subsets of correlated or aliased parameters (Li and Vu 2013). This implied that the columns of a sensitivity matrix associated with specific parameters were linearly dependent. And, where the correlation between parameters existed revealed a structural identification issue, which would need to be removed to be remedied.

The reparameterization approach included the following five steps: (1) conduct numerical identification analysis to determine the potentially unidentifiable parameters (Stigter, Joubert, and Molenaar 2017). This process would involve the construction of a full-ranked sensitivity matrix. Rank deficiencies indicated insensitivities between model output and input, these parameters would be unidentified (Reid 1977); (2) conduct symbolic identification analysis to pinpoint sets of totally correlated parameters. These symbolic calculations were conducted using a Jacobi matrix of the coefficients in a Fliess series expansion (Fliess 1981; Tunali and Tzyh-Jong Tarn 1987). As with the sensitivity matrix, a rank-deficient Jacobi matrix suggested the presence of zeros or a linear dependency in two or more matrix columns. This step would confirm the numerical findings from the first step; (3) define new model parameters which are solutions calculated in the previous step. In essence, this step computes the algebraic relationship between parameters which were confirmed as correlated (Choquet and Cole 2012); (4) replace model parameters in the original model with new ones, this step simplifies the original model by lowering its dimensionality in the removal of the correlated or unidentifiable parameters; (5) re-evaluate the structural identification of the reparameterized model by starting with different initial conditions to detect any further structural identification issues that may exist (Pia Saccomani, Audoly, and D'Angiò 2003).

The approaches outlined above are considered a-priori algorithms, in that they assess structural identification by the use of model definition. That being said, there are some a-posteriori approaches that use available data to detect parameters which are structurally non-identifiable. For example, one study applied *mean optimal transformations*, a non-parametric bootstrap-based algorithm to test the structural identification of model parameters (Hengl et al. 2007). Mean optimal transformations reveal the parameters which are functionally related, indicative of structurally non-identifiable parameters. The approach involved the performance of numerous fits to investigate non-parametrically whether the final parameter estimates form a low-dimensional manifold in parameter space.

Additionally, the construction of *profile likelihoods* has proved to be a successful method to assess identification (Murphy and Van Der Vaart 2000). This approach involved varying each model parameter around the maximum likelihood estimates and then reoptimizing the remaining ones. Profile likelihoods would reveal the dynamics of parameter identification; likelihoods that reached the upper and lower threshold of the confidence intervals were identifiable, whereas the nonidentifiable parameters yielded flat profile likelihoods. Plotting the other parameters along the profiled parameter would also reveal potential relationships with nonidentifiable ones (Raue, Kreutz, Maiwald, et al. 2009). The profile likelihood approach was extended to allow for the identification of parameter interdependence (Brastein et al. 2019). Though informative, this process of constructing profile likelihoods can be computationally demanding for larger systems because of the numerical reoptimization. To resolve this issue, a faster method to test identification without the need to calculate complete profiles using radial penalization was recently developed (Kreutz 2018).

Further, *Bayesian Markov Chain Monte Carlo* (MCMC) sampling has been proposed as a method to investigate structural identification. But in systems that are nonidentifiable, efficient mixing

and convergence of the Markov chains is difficult (Raue, Kreutz, Theis, et al. 2013). This problem could be cured by informative priors, though should only be implemented if they are based on actual insights and prior information.

Identification or identifiability has also been referred to as *equifinality* in the evaluation of process-based models (Guillaume et al. 2019). Generally, these models are purposed to directly inform policy recommendations so the quality of model output and capturing of uncertainty is a priority. Model outputs are dependent on the chosen model structure and parameterization (Van Vliet et al. 2016). And given the complexities of these models there exists multiple plausible model configurations that reasonably fit observed outcomes (Oreskes, Shrader-Frechette, and Belitz 1994). In other words, model inputs cannot be uniquely distinguished from the model output and under this condition, thus model behaviour represents a full range of indistinguishable plausible outcomes that may result in biased policy recommendations (Leclère et al. 2014). To conduct policy analysis on these types of studies the traditional 'best-fit' approach is utilised (Brown, Verburg, et al. 2013; O'Sullivan et al. 2016; Huber et al. 2018). An optimisation-based approach, Diverse Model Calibration for Robust Policy Analysis (DMC-RPA), was presented as a method to identify equifinal models and their implications on policy analysis (Williams et al. 2020). DMC-RPA contains two steps: (1) identify maximally diverse parameter sets that describe the structural characteristics that each match calibration data within a specified level of fitness, yet are as diverse as possible (DMC) (Brill, Chang, and Hopkins 1982; Zechman and Ranjithan 2004); (2) analyse the performance and consistency of policy effects over the equifinal model set (RPA); (3) choose the more robust model to inform policy. The main motivation behind the DMC-RPA approach rests with the argument, that due to the complexity of process-based models and data limitations, it is more instructive to accept the use of multiple "optimal" calibrated solutions, rather than a single solution. This would allow for the thorough exploration of the full parameter space and each solution would be selected based on their performance concerning modelled issues, whilst presenting as significantly different with respect to the decisions they specify.

6.2.3 Summary

Structural identification analysis involves the assessment of the structural equations of the model and can be undertaken without observational data. Practical identification analysis focuses on the ability to estimate parameters from observational data. That being said, when a model is structurally unidentifiable, this would imply the model was also practically unidentifiable. The reason is, that if model equations were structurally unidentifiable, then data elements, such as, the conditions of data collection conditions, data quality and quantity were redundant as without successfully determining the model structure it would not be possible to uniquely estimate parameters in practice. Furthermore, structural identification of a model would not imply practical identification because even if the model structure theoretically allows parameters to be estimated, there would still be the need for appropriate data to uniquely estimate parameters.

The methods outlined above are mathematical approaches to remedying practical and structural identification and they have a long history. The underlying assumptions which underpin the use of these traditional approaches however cannot be applied to complex ABM methodology e.g., linearity, equilibrium, normality, and insensitivity to initial conditions do not hold in complex systems e.g., non-linearity, out-of-equilibrium, no law of large numbers and path dependence/non-Markovian processes (Thurner, Klimek, and Hanel 2018).

Although practical and structural identification of the model parameters is equally important to the success of any model, the most challenging of the two to achieve in ABMs is structural identification. The challenge arises from the large number of parameters and structural assumptions characterising ABMs. As a result, properties of the macro-level cannot be explained directly from the properties of the micro-level (Giuseppe 2016). Due to stochasticity, feedback, and the non-analytical (i.e., no fixed, structural form) of ABMs, structural identification is extremely difficult. Compared to models that can be defined through a set of equations (i.e. identifying the relationship between the dependent variables and exploratory variables), in ABMs the relationship is implicitly defined through the numerical code (Giuseppe 2016); ABMs are mathematically intractable, thus rendering the traditional approaches to identification analysis redundant. Though difficult, structural identification should not be ignored as the very nature of ABMs, exhibits high degrees of path

dependence and non-linear dynamics, which could lead to significant implications if identification issues are not acknowledged (Windrum, Fagiolo, and Moneta 2007). An example of structural identification will be presented in the following section using the case study ABM.

6.3 Identification Analysis of Agent-Based Models

Chapter 5 presented the calibration results of the case study ABM using ABC. The ABC rejection method replaces the likelihood function by sampling and simulating the model with parameter values selected from a prior distribution. A set of summary statistics based on observed data would be derived and compared with the experimental data using a prespecified distance function. However, in cases such as these, where real data captured from a real-world system cannot be observed, synthetic data serves as a proxy. The distance function would produce a value and its size would indicate its proximity to that of the observed data. The results demonstrated how calibration could be used to successfully examine the parameter space and serve as a potential indicator of parameter identification issues. The vast majority of methods that exist in literature to determine and/or resolve identification issues all rely on the ability to analyse the model mathematically; concise methods for intractable models such as ABMs do not yet exist. That being said, the same SISa framework used to create the case study ABM was used to create an emotional contagion model using a set of ordinary differential equations (ODE) that could be analysed mathematically to demonstrate the parameter identification problem in its simplest form, in Chapter 4. The ODE model does not describe the case study ABM but rather is a simpler mathematical model that has similar characteristics when assuming homogeneity. This section will continue the investigation by first demonstrating how identifiability issues could arise in the parameter estimation process using the homogeneous emotional contagion ODE model. Following this demonstration, the same will be presented using pyABC as a tool on the case study ABM.

6.3.1 Structural Identification Analysis: ODE illustration

Parameter identifiability is often overlooked during the process of parameter estimation. As described earlier, structural identification of model parameters is achieved when a set of parameters can be uniquely estimated from a given model and real data (Kao and Eisenberg 2018). When there is non-identifiability this suggests there are multiple sets of parameter values that fit the model to data (Roosa and Chowell 2019). In other words, given a theoretical model of a phenomenon and specific input-output experiments, can parameters be uniquely determined? Chapter 4 first introduces the ODE model of emotional contagion, and here it will be used to demonstrate structural identification issues. The first case considers observing the stable equilibrium x_{+} to infer the rescaled parameters α and β . It is known that x_{+} satisfies

$$\alpha + (\beta - \alpha - 1)x_{+} - \beta x_{+}^{2} = 0, \tag{6.1}$$

which indicates that even if x_+ is known it would not be possible to directly estimate α and β , as they are both described by one equation. However, the relationship between the parameters can be investigated, by rewriting one in terms of the other. Here, the equation is rewritten for α in terms of β , giving

$$\alpha = \frac{x_+}{1 - x_+} - \beta x_+.$$
(6.2)

Figure 6.1 is a graphical illustration of Eqn. (6.2), which shows that even with full knowledge of x_+ , there are infinitely many pairs of α and β that would produce the same equilibrium value, thus a structural identification issue exists.

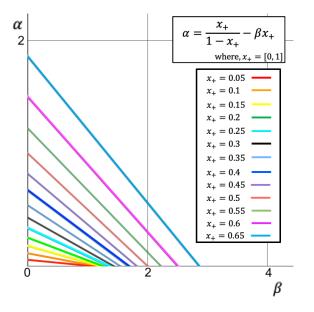


Figure 6.1: Plot of Eqn. (6.2) with different values of x_+

Essentially, Figure 6.1 illustrates different x_+ values and their corresponding lines given by equation Eqn. (6.2). In this regard, even if I_+ is known, the structural identification issue could

only worsen if an attempt is made to estimate the other parameters: a, g and N.

Further, if x_+ is known and for some time t, x(t) and \dot{x} is known, it could infer β and hence, α . To do this, substitute Eqn. (6.1) into Eqn. (4.8), to give

$$\dot{x} = \left[\frac{x_{+}}{1-x_{+}} - \beta x_{+}\right](1-x) + \beta(1-x)x - x$$
$$\beta = \frac{\dot{x}(1-x_{+}) + x - x_{+}}{(1-x_{+})(1-x)(x-x_{+})}$$
(6.3)

Now consider the case where the full evolution of I(t) is known (see Eqn. (4.14)), could *all* of the parameter values be inferred? Well, α and β could be inferred, but it would not be enough information to infer a, b, g and N.

Take the explicit solution Eqn. (4.13),

$$\frac{I - I_+}{I - I_-} = \frac{I_0 - I_+}{I_0 - I_-} \exp\left(-b(I_+ - I_-)t\right)$$

For given values of I_{\pm} , b and t, can different values of a, g and N produce the same values of I_{\pm} ? If so, there exists a structural identification issue.

From Eqn. 6.3, it is known that there are two numbers dependent on a, g and N. Let

$$\Delta = \frac{bN - a - g}{b}$$

and

$$\Gamma = \frac{aN}{b},$$

then I_{\pm} are fixed if Δ and Γ are fixed. Thus assuming that b, Δ and Γ are fixed, do these uniquely define a, g and N?

Note that for fixed b and Γ , a and N will need to be chosen such that

$$a = \frac{b\Gamma}{N}.$$
(6.4)

It follows that

$$\Delta = \frac{bN - a - g}{b},$$
$$= N - \frac{b\Gamma + gN}{bN},$$

when rearranged, can find

$$g = b\left(N - \Delta - \frac{\Gamma}{N}\right),\tag{6.5}$$

and so for fixed b and Γ , any choice of N such that a > 0 and is chosen according to Eqn. 6.4, and g > 0 and is chosen according to Eqn. 6.5 will give exactly the same evolution of I(t).

This outcome indicates a structural identification issue.

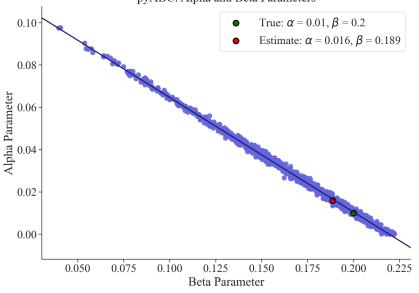
6.3.2 Structural Identification Analysis: ABM illustration

The previous section used the ODE emotional contagion model to demonstrate the structural identification problem. Models of complex systems, such as the one above, can be described in their functional form and thus be analysed for structural identifiability. But with computational models such as ABMs, which are mathematically intractable, the challenge lay in proving that ABMs can be affected by parameter identification issues, specifically the structural type. The ODE illustration demonstrated that even with the full knowledge of the steady-state equilibrium, infinitely many pairs of α and β would present the same equilibrium value. This section will present investigations into structural identification in both the homogeneous and heterogeneous configurations of the case study ABM.

To begin, the objective of this section was to reproduce the dynamics observed in Figure 6.1 but in the case study ABM. As previously demonstrated, calibration is an excellent tool to examine the parameter space and discover the existence of α and β pair values that would reproduce dynamics similar to that observed in the model output, the cumulative distribution. Parameter identification analysis should not be separated from the entire parameter estimation procedure but rather should be considered a significant step in the process. As calibration and identification analysis go handin-hand, this section uses pyABC as a structural identification detection tool. pyABC captures uncertainty and can be used as an indication of identification issues.

Homogeneous Configuration

Section 5.2 presented the calibration results for both the homogeneous and heterogeneous configurations. In the case of homogeneity, Figure 5.4 illustrated the evolution of α and β from uniformly distributed priors to defined posterior distributions; where the final population (No. of Populations, T = 11) is assumed to be the most improved posterior, attributed with the smallest ϵ . Each posterior distribution was made up of the accepted prior samples, in this case, 1000 particles. In the final posterior (No. of Populations, T = 11), each accepted particle presented with a cumulative distribution that was approximate to the true data. Ergo, pyABC was able to realise 1000 combinations of α and β values which presented the same equilibrium values, given some uncertainty. These 1000 potential combinations were visualised in Figure 6.2, with a line of best fit. In this figure, each dot represents a particle that forms the final posterior (No. of Populations, T = 11).



pyABC: Alpha and Beta Parameters

Figure 6.2: Homogeneous Config: Accepted Particles in Final Population

pyABC Algorithm Output		
Parameter	True Values	Posterior Modes
α	0.01	0.01595468
β	0.2	0.18851214
Summary Stat: Average	534.104	535.318213

Table 6.1: Summary Statistic Comparison from Parameter Values

For reference, the true α and β values are annotated in green, and pyABC posterior modes or parameter estimates are annotated in red. The most interesting observation of this figure comes from the line of best fit and its expression of a linear relationship similar to the dynamics uncovered from the analysis of the ODE emotional contagion model in Figure 6.1.

Figure 6.2 effectively demonstrates the existence of structural identifiability issues in the homogeneous configuration of the case study ABM; as each accepted particle could be interpreted as a potential combination of α and β parameter values that could produce results similar to the true model output i.e., the cumulative distributions of the Number of Infected Agents per Iteration.

However, when considering the success of parameter estimation, the pyABC process produces posterior distributions from the final population to predict and forecast. This is considered a successful implementation. Yet, success should also be determined by a lack of errors that arise during the implementation of the algorithm and the accuracy of the posterior mode. Nonetheless, in this case, as the true values are known, the distances or proximity between the summary statistics and true and estimated parameter values are observable close (See Table 6.1) which indicates success. That being said, it is worth noting that the *Average* Number of Infected, the summary statistic, was not as exact.

In addition to this, Figure 6.3 presents the evolution of the posterior distributions from the initial population to the final posterior, which is considered the most improved. This comparison demonstrates the effective iterative pyABC process and convergence around both the true and estimated parameter values.

Moreover, this figure illustrates the density of accepted particles which form the initial and final posterior distributions. The area of the parameter space characterised by the lightest hue is a high-density area; in other words, most particles are concentrated within this area. More noticeably, the identifiable parameter space has contracted through the populations and by T = 11, the estimates (posterior modes) sit centrally on the line of best fit. This is indicative of the unique determination of α and β values from all the other potential combinations. Therefore, the homogeneous configuration parameters of the case study ABM are structurally identifiable.

CHAPTER 6. IMPACT OF HETEROGENEITY: PARAM-ETER IDENTIFICATION

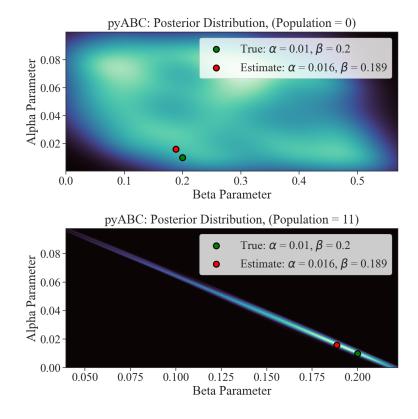


Figure 6.3: Homogeneous Config: Initial and Final Posterior Distribution

Heterogeneous Configuration

To introduce heterogeneity, the Number of Agent Groups was increased from one to two groups. Table 5.3 summarises the input used to initialise the pyABC algorithm and Figure 5.9 illustrates the evolution of the posterior distribution through the populations, the accompanying posterior modes and estimation analysis were summarised in Table 5.4 and Figure 5.11, respectively.

Figure 5.9 presents the convergence around the true $\beta_{\text{Group 1}}$ and α values, but not very well around $\beta_{\text{Group 2}}$. And as with the homogeneous case, the 1000 potential combinations of $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$ were visualised in Figure 6.4. Unlike the ODE model and the homogeneous configuration, Figure 6.4 presents a non-linear relationship between the β parameters.

6.3. IDENTIFICATION ANALYSIS OF AGENT-BASED MODELS

CHAPTER 6. IMPACT OF HETEROGENEITY: PARAM-ETER IDENTIFICATION

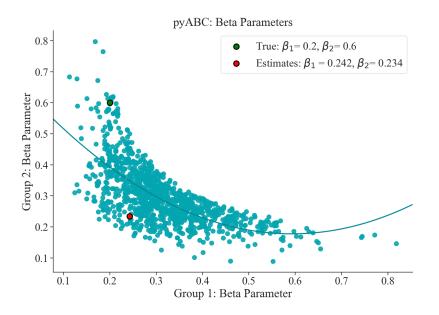


Figure 6.4: Heterogeneous Config: Accepted Particles in Final Population for Beta Parameters

Yet it proves that pyABC was able to identify 1000 other combinations of $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$, which can reproduce similar dynamics to that observed in the model output. Table 6.2 presents the true and estimated values, as well as the summary statistic. Although the posterior mode for $\beta_{\text{Group 2}}$ is significantly lower than the true value, the summary statistic of the model output is incredibly close. This suggests, that though the parameter estimation process was successful, there exists a structural identification issue.

pyABC Algorithm Output		
Parameter	True Values	Posterior Modes
α	0.01	0.01850757
$eta_{ ext{Group 1}}$	0.2	0.24232129
$eta_{ ext{Group 2}}$	0.6	0.23383305
Summary Stat: Average	700.173	699.732148

Table 6.2: Summary Statistic Comparison from Parameter Values

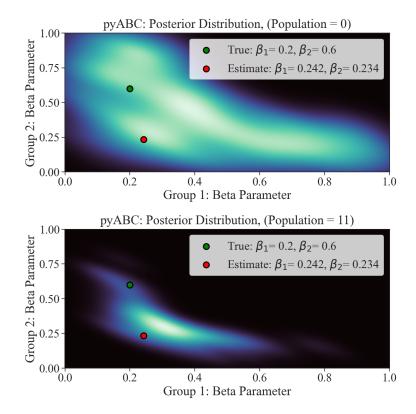


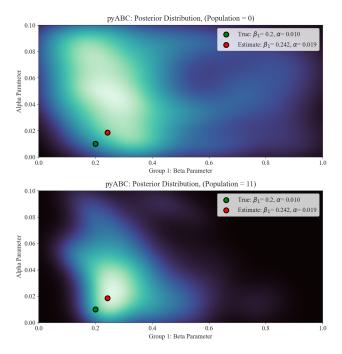
Figure 6.5: Heterogeneous Config: Initial and Final Posterior Distribution

Figure 6.5 presents the evolution of initial and final posterior distributions of the β parameters. As seen previously, the area with the lightest hue is characterised by the highest number of particles by potential combinations of $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$ which would reproduce dynamics observed in the model output. Although the posterior modes are near the concentrated area, it is a notable distance from the true values. The question of how unique the model inputs are is worth considering, as even after changing β values (see Appendix C.2), the posterior modes were almost always relatively identical. Introducing heterogeneity through α presented the same issue, pyABC failed to produce distinct estimate values for both α parameters (see Appendix C.1). Given these observations, evidently, the introduction of heterogeneity impacts the structural identifiability of the model.

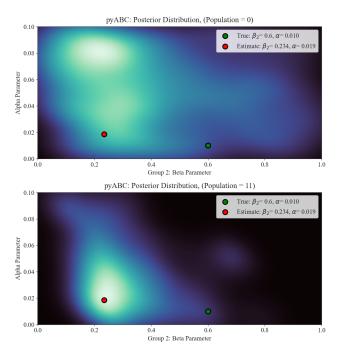
Furthermore, Figure 6.6 presents the evolution of the initial and final posterior distributions of the α and β parameters.

6.3. IDENTIFICATION ANALYSIS OF AGENT-BASED MODELS

CHAPTER 6. IMPACT OF HETEROGENEITY: PARAM-ETER IDENTIFICATION



(a) Heterogeneous Config: α and $\beta_{\text{Group 1}}$ Posteriors



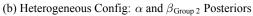


Figure 6.6: Heterogeneous Config: Initial and Final Posterior Distributions

Figure 6.6a presents the posterior distribution of α and $\beta_{\text{Group 1}}$. Unlike the homogeneous configuration, there is no observable linear relationship between the parameters. Instead, the pyABC iterative process reduces the parameter space and converges towards the pyABC estimate, which falls into the lightest hue of the high-density area. pyABC only slightly overestimates α and $\beta_{\text{Group 1}}$, as the values are approximate in the second and first decimal points respectively. Although parameter estimation is successful and the true value sits on the cusp of the high-density area, there is evidence of a structural identifiability issue.

Similarly Figure 6.6b presents the posterior distribution of α and $\beta_{\text{Group 2}}$. There is some clear convergence around the pyABC estimates but the true values fall dramatically outside of the high-density area. Also, the distance between the true and estimated is considerably large. These findings indicate a structural identifiability issue. pyABC estimates of $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$ are near approximates; it is possible that pyABC is unable to distinguish between the effects of two β parameters in the data, even though they are distinct. Thus, pyABC was unable to uniquely determine $\beta_{\text{Group 1}}$ from $\beta_{\text{Group 2}}$.

A final yet notable finding is that α remains structurally identifiable as in the Homogeneous Configuration, it consistently remains within the lightest hue of the high-density area.

The implications of these unresolved structural identification issues presented in the β parameters will be further explored in the following section.

6.4 The Implications of Unresolved Structural Identification Issues

This section will begin by first presenting an example in which failing to address structural identification issues may impact agent-based model results; before further discussing the implications.

6.4.1 Unresolved Structural Identification Issues: An Illustration

Pandemics have had unprecedented catastrophic implications on the health, social and economic well-being of the global community, as proven by the Coronavirus disease 19 (COVID-19) (WHO 2019). Vaccine development is typically a long, complex process, often lasting 10-15 years (Rappuoli, Black, and Bloom 2019), but COVID-19 vaccines were developed in under a year. With this rapid research development, the public grew concerned that the speed of development must have compromised the vaccine safety in some way. With these concerns came vaccine hesitancy.

Vaccine hesitancy is not a new problem it is a long-standing problem, that urgently needs to be addressed with care and tact (Chadwick et al. 2021). Vaccine hesitancy in the UK is a compounded issue and is connected to the long-term decline of trust in public and private institutions (Devine et al. 2021); but from the start of the global pandemic, there was a range of disinformation and conspiracy theories about the origins and severity of COVID-19 spread online and on personal messaging platforms, partially undermining policy on social distancing (Miller 2020; Freeman et al. 2022). Ultimately these misconceptions regarding vaccine safety and efficacy undermine the long-term goal of total population immunity (Thunstrom et al. 2020).

Vaccine hesitancy can be contagious and the associated attitudes of an individual's network can influence another's decision to vaccinate (Konstantinou et al. 2021). This phenomenon is known as Social Contagion as described in Chapter 3.3.2; whereby the spread of affect from Person A (the initiator) to Person B (the recipient) is defined as *emotional* contagion. Attitudes and ideas towards vaccination can disseminate through networks and an individual can adopt and demonstrate behaviours modelled by another person they are connected to (Christakis and Fowler 2010, 2013; Karashiali et al. 2023).

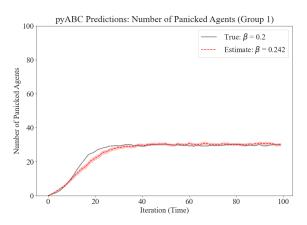
As vaccine hesitancy is a social information problem, the success of any vaccination programme

depends on where and how information about vaccine safety and efficacy is disseminated. Thus, public opinion research specifically into uncertainty suggests some people who have not yet formed firm opinions may be receptive to gaining information and some may find that new information resolves any ambivalence (Conner and Sparks 2002; Berinsky 2006). Therefore, identifying what explains the social endorsement of vaccines can help inform a non-coercive approach (Giubilini et al. 2019; Vanderslott 2019). Studies into misinformation have suggested that older adults are significantly more susceptible to it than younger adults (Mitchell, Johnson, and Mather 2003; Davis 2014). When it comes to mitigating or correcting the effects of vaccine hesitancy with new information through social endorsement, strategies must accommodate socio-demographic groups and their susceptibilities. Thus the question of which groups to first prioritise is critical.

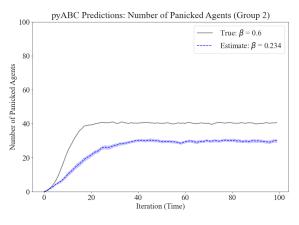
Consider this very example as the heterogeneous scenario explored in Subsection 6.3.2. Hypothetically, $\beta_{\text{Group 1}}$ could represent the transmission rate of vaccine hesitancy in older adults and $\beta_{\text{Group 2}}$ represents the transmission rate in younger adults, as summarised in Table 6.2. Table B.2 presents the observed data. As the true β values would be unknown for each group, pyABC would be implemented to construct posterior distributions from which samples for β are drawn and predictions made, which policymakers could use to develop policies to mitigate the effects of panic around vaccine hesitancy. The posterior distributions effectively capture any uncertainty associated with these predictions (Ferguson et al. 2020). In this example, Figure 5.9 are pyABC posteriors for $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$. Failing to structurally identify the parameters means that the samples from which $\beta_{\text{Group 2}}$ values are drawn will underestimate the true rate of transmission in younger adults.

For this illustration, the ABM output, *Average* Number of Panicked Agents, is calculated using the posterior modes in Table 6.2, over 100 iterations. Standardly, ABM output is estimated by sampling values from the posterior distributions and using the average values as the estimated parameter value.

CHAPTER 6. IMPACT OF HETEROGENEITY: PARAM-ETER IDENTIFICATION



(a) Number of Panicked Agents in Group 1 (Older Adults)



(b) Number of Panicked Agents in Group 2 (Younger Adults)

Figure 6.7: Comparison between True and Predicted Number of Panicked Agents over 100 iterations

Figure 6.7 compares the predicted Number of Panicked Agents in Older Adults (Group 1) and Younger Adults (Group 2), respectively. Figure 6.7a presents little deviation between the predicted Number of Panicked Agents in the true and estimated simulations.

Whereas predictions made with the structurally unidentifiable parameter as seen in Figure 6.7b, present significantly different dynamics in the predicted Number of Panicked Agents. Now, considering the task of information dissemination regarding vaccine safety and efficacy to mitigate the effects of panic, policymakers must decide on how to appropriately target each age demographic.

To do this, policymakers would need to identify susceptibility to panic for each age demographic: this information is drawn from pyABC predictions of the Number of Panicked Agents and not the true data. As the dynamics of each β estimate in Group 1 and Group 2 are indistinguishable, policymakers may incorrectly assume that age does not affect the Number of Panicked Agents in their population. Rather than appropriately targeting each age demographic with tailored social endorsements according to their susceptibility to panic, policymakers may choose not to prioritise either group. In doing so, policymakers fail to consider the impact younger people have on disease transmission and will counteract efforts made to manage vaccine hesitancy perpetuated by the spread of panic.

6.4.2 Unresolved SI Issues: A Discussion

Although the example above is hypothetical and incredibly simplified, it presents a strong argument for a very real and critical issue in ABM research. It cannot be reiterated enough times: parameter identification is fundamental to the success of parameter estimation. Uncovering identification issues is equally as important as conducting sensitivity analysis and each procedure reinforces the other. Failure to identify parameters in ABMs is common but can be spotted with the same crossvalidation tests as demonstrated by Carrella (2021). Carrella (2021) compared the performance of 9 parameter estimation algorithms across 41 models and found no single algorithm was the best for all or even most of the models.

Most especially resolving identification issues analytically remains an arduous task for mathematically tractable systems and is yet to be accomplished in intractable systems. For systems such as these, it is important to explicitly acknowledge and document the influence of identification on the modelling process, and how they have been recognised (Guillaume et al. 2019).

Given the stochastic nature of ABMs, there is some uncertainty involved in the simulation process. That being said, when calibrating the model with the chosen algorithms different runs should not return different parameter value estimates. And though trivial, the modeller should repeat the calibration process with different initialisations, ideally with randomly selected initial parameter values, to check if it returns unique values for parameters (Shin et al. 2015). ABMs are microscale models which simulate the simultaneous interactions of multiple agents, usually to reproduce dynamics observed in real-world systems (Gustafsson and Sternad 2010). Nonetheless, discussions and proposals for ABMs as predictive tools, have begun to form (Chattoe-Brown 2023). If the model is structurally unidentifiable, then the model cannot be used for predictive analysis. Failing to uniquely determine the input from output during parameter estimation or calibration will lead to inaccurate predictions as key behaviours of the system were not captured during model development (Williams 2011). However, there has been some debate about prediction in the ABM literature and its utility (Elsenbroich and Polhill 2023).

Polhill, Hare, et al. (2021) presented path dependency as a contributing factor to inaccurate ABM predictions due to the intractability of exhaustively searching the space of models that might match the available data. Though they emphasise that there are other purposes for ABMs beyond prediction, and even if the predictions are considered inaccurate there is still some predictive utility in being able to detect transitions between states in the real world as observed in the model.

While non-identification indicates a lack of appropriate information to choose between alternative models, in practice the "right" information may take a considerable length of time to obtain, or may never be available at all (Rothenberg 1971). So, depending on the necessary predictions, having multiple plausible models may not be of any consequence as differences in prediction may be small enough to be acceptable, or able to be addressed by decision-makers through adaptive management.

Regardless of the response to identification analysis, the modeller bears the responsibility of transparency about their source and treatment of identifiability. The modeller should include documentation that describes whether model parameters have been parametrically identified and how it was assessed. If the model parameters were non-identifiable, the documentation should describe the anticipated consequences and the responses undertaken.

But why does all this matter, especially if calibration is successful? Well, the implication of unresolved structural identification issues depends on the purpose of the empirical ABM: is the model's purpose exploratory or predictive? Edmonds et al. (2019) presents a robust review of the different purposes for a simulation model of complex social phenomena. An exploratory ABM

allows for unbounded experimentation as the output is simply meant to educate and broaden understanding of a target system. But even in this case, a structural unidentified model means that the modeller may not necessarily learn the right or relevant information about the model. Whereas an ABM built for predictive or forecasting power is made to inform and govern the target system in the real world (Chattoe-Brown 2023). Therefore, ensuring this type of ABM is structurally identifiable directly impacts the accuracy of the forecasts which will impact real-world social policy. As seen in the example above, the ability to correctly and uniquely determine the β values for each Agent Group is detrimental to the success of the ABM and its predictive utility. Naturally, it is important to consider that the true values of the models are unknown in the real world and so the impact of identification issues may not be so apparent to modellers. This is why implementing some of the above guidelines in the course of their research, may help bring to light this issue and reevaluate the strength and purpose of the ABM.

6.5 Summary - Parameter Identification

This chapter began by presenting the issue of parameter identification. Section 6.2 outlined the two types of identification: practical and structural identification and the traditional analytical approaches taken to remedy unidentifiability. Here, Structural identification was defined as the process of uniquely determining model input from any given model output. As there is seemingly little research on structural identifiability in ABM, this study aimed to establish the existence of this problem, particularly as the result of increasing heterogeneity. Thus, Section 6.3 demonstrates structural identification issues in the ODE model of the emotional contagion ABM used as a case study in this thesis. Using calibration as a tool, specifically pyABC, the results demonstrated that the introduction of heterogeneity had the potential to impact the structural identification of the model. And lastly, Section 6.4 considered the implication of unresolved structural identification issues in ABMs.

Chapter 7

Conclusion

Contents

7.1	Chapter Overview
7.2	Summary of Results
7.3	Evaluations
7.4	Recommendations for Future Work
7.5	Concluding Remarks

7.1 Chapter Overview

Chapter 1 presented a set of research objectives. These objectives were as follows:

- 1. Review and discuss the literature related to ABMs, with a focus on heterogeneity as a characteristic. Also, briefly review the literature on emotional contagion and compartmental models to facilitate the design and development of the case study model.
- 2. Design and build the case study ABM, simulating the transmission and infectiousness of emotional contagion. Then determine optimal values for the ABM using sensitivity analysis.

- 3. Evaluate the ABM by assessing its response to varying parameter values using calibration to examine the parameter space.
- 4. Define and investigate the problem of parameter identification in heterogeneous ABMs.

The overarching aim of this study was to investigate heterogeneity in ABMs and it proposes parameter identification as a potential impact. This study sits within a relatively new field of research and as there exists no established method to investigate parameter identification in ABMs, it is important to consider the constraints of this experiment. However, this study has shown that structural identification arises in ABMs, particularly as the direct result of heterogeneity in Chapter 6.

This chapter marks the conclusion of the investigation and will summarise the results of the work undertaken thus far to satisfy the aims and objectives of this thesis. Further, this chapter will include an evaluation of the results and some recommendations for future work.

7.2 Summary of Results

This section aims to summarise the results of this study and in doing so addresses objectives 1, 2, 3 and 4.

Chapter 2 presented ABMs as a method for modelling complex systems. Its popularity is accredited to its flexibility in application which effectively captures the presence of heterogeneity in a system. This chapter defines heterogeneity as agent granularity, referring to the *coarseness* of descriptive attributes and behaviours assigned in the agent component (Gao, Song, and Wang 2013). This chapter also considers the impact of heterogeneity in ABM literature, in the examination of comparative homogeneous and heterogeneous scenarios spatial. The following observations were formed: *i*) agent heterogeneity is often displayed in two non-mutually exclusive forms: the categorisation and/or variability of the agent population and attributes, *ii*) agent heterogeneity is extrinsic, in that heterogeneity is initialised into a model but the evolution away from the initial heterogeneity is rarely monitored. Heterogeneity which develops outside of the initial conditions is referred to as generated heterogeneity, *iii*) the variable used to demonstrate agent heterogeneity can impact model results, *iv*) undetected pre-conditions between components can affect the impact of agent heterogeneity, *v*) the object of study and research purpose are contributing factors to deciding between imploring homogeneous or heterogeneous assumptions, *vi*) If agent interactions generate network effects, then the types and effects of heterogeneity found in network sciences apply to agent-based models. Two types of heterogeneity found in network sciences are structural and relational heterogeneity. Structural refers to the different structural changes that arise as a direct result of agent heterogeneity; relational heterogeneity emerges directly from agent interactions and finally, *vii*) Comparative homogeneous and heterogeneous scenarios should be a standard, to help evaluate the impact heterogeneity has on the system being modelled. Modelling heterogeneity may be a computationally expensive task, but in some cases has been made unnecessarily so; thus it is important to discern when the increased granularity no longer enriches the model's explanatory or predictive powers.

Chapter 3 presents the literature used to build a theoretical understanding of emotional contagion as a form of collective behaviour. This chapter began with an outline of a range of definitions and forms of collective behaviour. More specifically, emotional contagion was defined generally as the transmission of emotion between individuals. This chapter also presented two methods for modelling emotional contagion: compartmental models and information diffusion models. This chapter provided literature on compartmental models which facilitated the design and development of the case study ABM in Chapter 4. Chapter 2 and Chapter 3 addressed objective 1.

Chapter 4 presented the simple ABM based on the SISa model framework outlined in Chapter 3. It presented the dynamics of the homogeneous configuration by fixing the Agent Parameters: α , β , γ and Number of Agent Groups, whilst varying the Model Parameters: Number of Agents, Number of Iterations and Model Instances. Then, heterogeneity was introduced by increasing the Number of Agent Groups. The dynamics of the output in the homogeneous and heterogeneous configurations were compared and found to be fundamentally similar. Some sensitivity analysis was conducted to investigate the impact of Agent Parameters on the output, whilst fixing the Model Parameters. From this, parameter values were identified which could be considered optimal based on the effect on the output: in summary, the impact of α was most observable when small, whilst β and γ were most effective when larger. This chapter addressed objective 2.

Chapter 5 included a series of calibration exercises undertaken to explore the parameter space of the case study ABM. The purpose of this was to investigate the impact of heterogeneity, which could materialise as a parameter identification problem. The simple approximate Bayesian computation (ABC) exercises presented significant results for both the homogeneous and heterogeneous configurations. This was observed in the defined peaks which characterised the α and β posterior distributions. This chapter addressed objective 3.

Lastly, Chapter 6 presented the issue of parameter identification. It outlined the two types of identification: practical and structural identification, as well as the traditional analytical approaches taken to remedy unidentifiablity. This study defined structural identification as the process of uniquely determining model input from any given model output. Though the research area was small, this study aimed to establish the existence of this problem, particularly as the result of increasing heterogeneity. This chapter first illustrated structural identification issues in the emotional contagion ODE model and was later able to present the same issue in the case study ABM using pyABC. This chapter demonstrated that the introduction of heterogeneity, even on a small scale, had the potential to impact the structural identification of model parameters. This chapter addressed objective 4.

In light of the above summary, the main contributions of this thesis are:

- This thesis proposes a specific definition of heterogeneity in ABMs for which its impact can be measured. Heterogeneity is limited to the agent component and is defined as agent granularity; which refers to the coarseness of descriptive attributes and behaviours assigned in the agent component e.g. the number of model parameters used to describe the agent class. This definition was proposed following the detailed literature review in Chapter 2, which comparatively reviews homogeneous and heterogeneous scenarios in agent-based models.
- 2. This thesis proposes the impact of modelling heterogeneously in ABMs is parameter nonidentification. This study demonstrates the existence of parameter identification issues in heterogeneous ABMs and how they can be detected using approximate Bayesian computation calibration. To establish parameter identification issues as a potential impact of heterogeneity in ABMs, this study first considers the concept of parameter identification. Chapter 5

defines parameter identification and uses a case study model of emotional contagion introduced in Chapter 4 to prove its existence analytically (using the emotional contagion ODE model) and computationally (using the emotional contagion ABM).

3. Parameter identification i.e. the ability to identify a unique set of parameter values that produce a particular model output, should be included in the standard ABM calibration process. This thesis proposes: that to successfully calibrate an ABM should go beyond presenting a single parameter point or capturing uncertainty by presenting a selection of best-fitting parameters, and go a step further by uniquely distinguishing the model input from the given output. This was demonstrated in Chapter 6, which used approximate Bayesian computation calibration not only to achieve parameter estimation but also to examine the wider parameter space and determine whether the estimated parameters were uniquely identified from the model output.

7.3 Evaluations

The purpose of this section is to evaluate the results of the investigation, which will determine key areas for future work and development. This study ascertains that an impact of heterogeneity is parameter identification, specifically the structural type. Before investigations into identification, the first challenge lay in simply defining agent heterogeneity and understanding its broader impact on ABM research. This study had to limit the definition of heterogeneity and could only consider a specific type, namely animate agent objects. A shortcoming of this approach is potentially the oversimplification of a massively complex phenomenon, which most definitely would influence the course of this investigation. Though it may be considered a rudimentary step, formulating such a precise definition was crucial in developing the working framework of the research study.

Having established a definition for heterogeneity, the next task was to select a sufficient method to model emotional contagion. Compartmental models of infectious diseases were the ideal choice due to their widespread use and application, as well as their analytical tractability. However, the SISa framework was used because it could model a topic of interest, namely emotional contagion, and could be represented analytically using tractable ODEs (to help inform intuition about model dynamics and parameter identification) and as an ABM through which heterogeneity could be incorporated. Though successful, it is important to note that the simple model may not sufficiently capture the full complexity of parameter identification in ABMs. This study aimed to examine the impact of heterogeneous models which often contain too much information to explain the dataset, but this study does not support the use of homogeneous models if they too fail to adequately describe the dataset. Thus, this study urges modellers to consider the number of heterogeneous parameters they include in their ABMs. In limiting heterogeneity to a small number, specifically $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$ the computational running times were constrained. Attempting to fit many more parameters would have made the task numerically difficult. However, the heterogeneity captured with two β parameters may not be an adequate sample for this study. Thus findings are limited and cannot be extrapolated. Increasing the model complexity through the addition of heterogeneous parameters could also impact the results of the structural identification analysis attained in this study.

A further challenge lay in defining structural identification. Though more established in literature than practical identification, the difference between the two types is not particularly distinct. This study assumes practical identification issues arise from the experimental conditions and model structures and as a consequence creates variation in parameter estimates. Whereas structural identification focuses primarily on model structures which create variation in the estimates. Both of these concepts exhibit a great deal of overlap, especially in the proposed methods used to remedy the issue. Some additional work is needed to establish whether the two types should simply be merged or made more distinct.

Research into detecting and remedying structural identification in ABMs is relatively new. There are no widely accepted approaches to apply. So, to undertake this experiment the inverse problem approach was utilised and calibration was used as a tool. The case study ABM produced a synthetic dataset which was used as a substitute for real data. As synthetic data was used, investigating the practical identifiability of the parameters would be ineffectual. However, the parameter that was selected to introduce heterogeneity was of the most importance, as introducing an additional parameter to the ABM changes the model structure which was the object of study. It is important

7.3. EVALUATIONS

to consider the significance of the chosen parameter i.e., would structural identification present in the same way, if heterogeneity was introduced in α or γ , rather than in β ? This is a critical question as each parameter played a specific role in the spread of emotional contagion and thus would have distinguishable impacts on the model structure. Although there is an indication of a structural identification in β , this may not hold in the case of multiple α or γ parameters.

A further shortcoming lay in the choice of calibration method, as the chosen method affects the efficacy of the parameter identification analysis. As emphasised by Carrella (2021) made significant contributions to this field of study: they compared the performance of 9 parameter estimation algorithms across 41 ABMs and found that no single algorithm was the best for all or even most of the models. Furthermore, using rank estimation algorithms they determine model identifiability. The model would be classified as unidentifiable if all 9 algorithms fail to achieve cross-validation performance above a threshold then the parameter cannot be identified. They used two performance thresholds: where the best performance among all algorithms was less than 0.1 known as "serious identification failures" and when the best performance was below 0.3 this was referred to as "identification failures". They conclude that identification failure or unidentifiability is common in ABMs but can be determined through cross-validation tests.

In this study, ABC was selected as it is considered the most robust and successful calibration method, though can be used to conduct identification analysis some improvements could be made. There is a need for an established method for parameter identification in ABMs, as simple differences in how modellers implement or initialise the ABC algorithm could yet influence the identification results. As previously indicated by Polhill and Salt (2017), determining ABM performance should consider more than just the model fitness. They suggest paying more attention to expressivity of a formal language for ABM ontologies. Expressivity refers to the logic behind the axioms used to freely create, whilst maintaining decidable reasoning. Thus modelling approaches can be compared according to their ontological expressivity which captures descriptions of the model states. Expressivity in ABMs refers to classes, inheritance, individuals, data properties, object properties, lists, arrays, domains and ranges needed. Due to the very flexible nature of ABMs ontology is largely subjective, but there is still value in knowing how 'good' the subjective choice is.

Polhill and Salt (2017) propose assessing ontologies in the following ways: logical consistency, populating it with instances, stakeholder and/or expert evaluation and comparison with existing ontologies. That being said, even though ABC was used to calibrate the emotional contagion ABM, there exist other validation methods to determine model quality that could be used to evaluate parameter spaces and model identifiability.

7.4 **Recommendations for Future Work**

Having offered some critique of this investigation in the previous section, this section contains some proposals for future work which might expand upon what has been formally presented in this thesis. The larger goal for this field of study should lie in constructing an appropriate definition of structural identification in ABMs. A distinct definition would come with clearer indicators for which to detect potential identifiability issues. From that point only, can a suitable method to resolve the issue form which goes beyond the process of cross-validation.

Following on from the research undertaken in this study, smaller more incremental steps can be made towards achieving this goal. The first of which is a further examination of heterogeneity expressed in α and γ . As mentioned previously, it is important to establish the effect each parameter could have on the output to gain certainty in identification analysis. Additionally, increasing the number of parameters is pertinent to achieving a degree of certainty in the results obtained from identification analysis.

Furthermore, this study compared the homogeneous and heterogeneous configurations of the emotional contagion model in Chapter 2.3. This exercise indicates that closing the distance of the Average Number of Infected between Homogeneous and Heterogeneous Configurations could be achieved by purposefully selecting combinations of β values which reflect the approximate Average Total Number of Infected values. An extension of this study could be to investigate the potential equivalence between the model configurations.

Another way in which this investigation could be expanded upon is by exploring the choice of compartmental models. The SISa framework is adequate but may be too simplistic to capture the complexity of heterogeneity. These frameworks feed into the construction of the ABM and therefore directly impact the structural identification of model parameters.

A final way to improve and expand this study is through a comparative study of calibration tools as detection for identification analysis. As mentioned in Chapter 6, calibration and identification analysis cannot be separated as they are interdependent. However, results from Chapter 5 suggested caution should be exercised in the use of current calibration methods as an effective tool. That being said if the study into ABC as a tool continued, then there lay potential in attempting to measure the high-dense areas in the posterior joint distributions. This area would be an indicator of what is considered the identifiable zone within the parameter space.

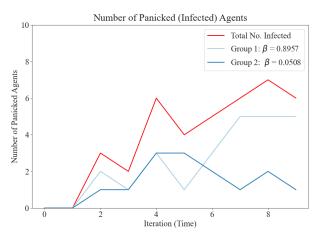
7.5 Concluding Remarks

This chapter provides an overview of the results of the investigation presented in this thesis, noting the limitations and recommendations for future research. This study has presented parameter nonidentification as a potential impact of heterogeneity in ABMs. This research serves as a motivation to the wider ABM research community, to encourage further work into this new field. Whilst this investigation has been successful, there remain fundamental challenges that need to be addressed. In addressing these limitations, there is hope for an established and widely accepted method for both the detection and resolution of structural identification issues which may arise in empirical agent-based models, such that practitioners and policymakers can utilise agent-based models with greater confidence and certainty in model results.

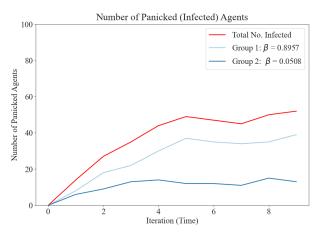
Appendix A

Chapter 4

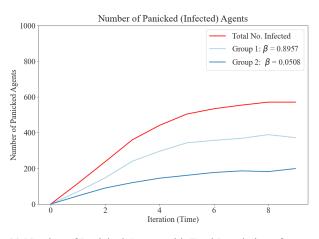
This Appendix presents Figures of the Number of Infected in the exploration of Heterogeneous Configuration in Chapter 4.



(a) Number of Panicked Agents with Total Population of 10 Agents



(b) Number of Panicked Agents with Total Population of 100 Agents



(c) Number of Panicked Agents with Total Population of 1000 Agents

Figure A.1: Number of Infected with an increasing agent population over 10 iterations

Appendix B

Chapter 5

This Appendix describes the Observed Data already seen in Chapter 4, that will be used in the model calibration.

B.1 Homogeneous Config. Data

Homogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	1000	
Single Instances	1(t)	
Number of Agent Groups	1	
α	0.01	
β	0.2	
γ	0.1	

Table B.1: Homogeneous Configuration Parameter Values: Observed Data

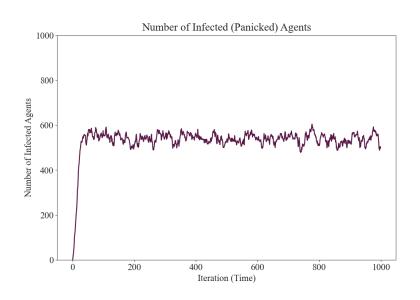


Figure B.1: Number of Infected

B.2 Heterogeneous Config. Data

Heterogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	1000	
Single Instance	1(t)	
Number of Agent Groups	2	
α	0.01	
$eta_{ ext{Group 1}}$	0.2	
$eta_{ ext{Group 2}}$	0.6	
γ	0.1	

Table B.2: Heterogeneous Configuration Parameter Values: Observed Data

B.2. HETEROGENEOUS CONFIG. DATA

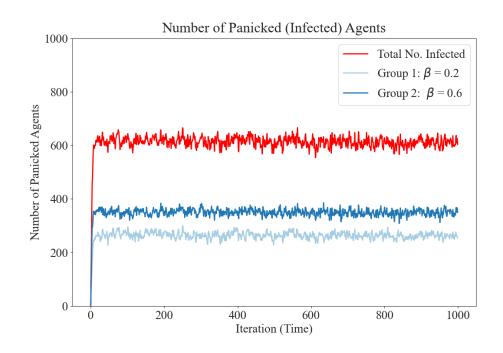


Figure B.2: Heterogeneous Configuration: Number of Infected

B.3 Approximate Bayesian Computation Exercise: Constrained Pri-

ors

This section contains the results of the ABC exercise in which the prior were constrained.

B.3.1 Homogeneous Config.

pyABC ABC-SMC Algorithm Input: Constrained Priors			
Parameter	Value		
Data	CDF (Number of Infected)		
Distance Function	RMSE		
Max. No of Populations	12		
Population Size	1000		
Epsilon (ϵ)	Unspecified		
α	U(0.01, 0.05)		
β	${\cal U}$ (0.0, 0.4)		

Table B.3: pyABC ABC-SMC Algorithm Input: Heterogeneous Configuration

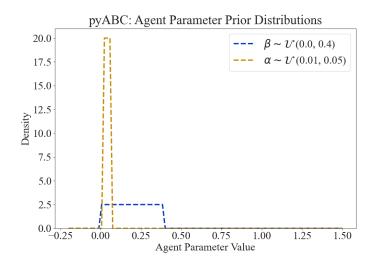


Figure B.3: pyABC Constrained Priors: Alpha and Beta Parameters are Uniformly Distributed

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

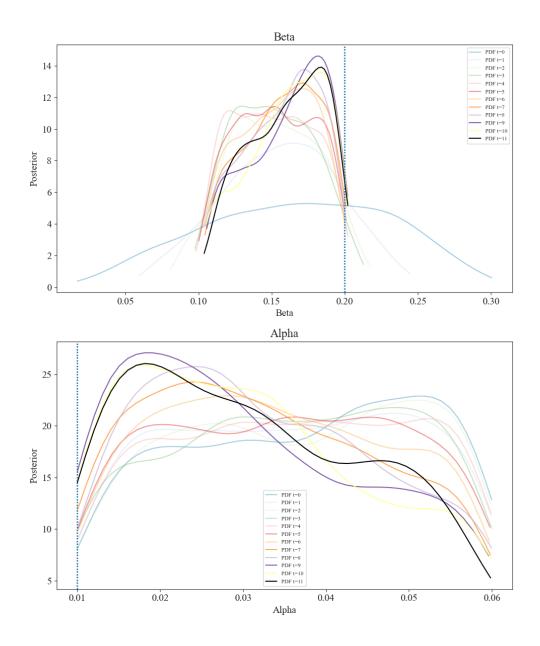


Figure B.4: pyABC Posteriors: Conditional Probability of Alpha and Beta Parameters

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

pyABC Algorithm Output: Posterior Modes			
No. of Populations	Mode		
No. of Populations	α	eta	
0	0.05182242	0.17333339	
1	0.04777098	0.16533711	
2	0.0506588	0.13098779	
3	0.04875285	0.13049924	
4	0.05276988	0.12174599	
5	0.03644685	0.15099122	
6	0.02836106	0.17095419	
7	0.02425427	0.17129444	
8	0.02429455	0.17147166	
9	0.01812292	0.18238673	
10	0.01816963	0.18468046	
11	0.01815208	0.18410205	

pyABC Algorithm Output: Posterior Modes

Table B.4: pyABC Output: Posterior Mode of α and β

APPENDIX B. CHAPTER 5

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

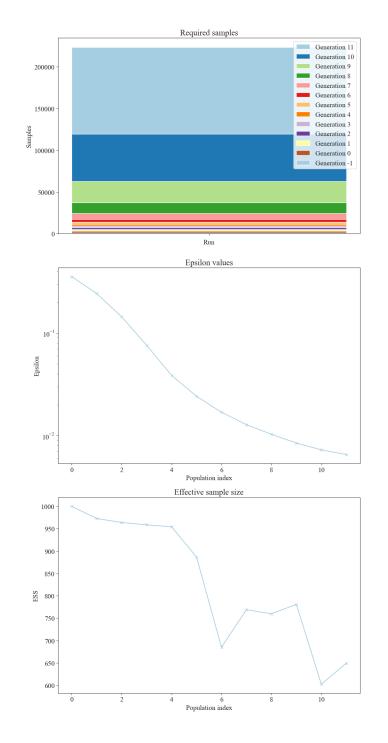


Figure B.5: pyABC Priors: Alpha and Beta Parameters are Uniformly Distributed

B.3.2 Heterogeneous Config.

pyABC ABC-SMC Algorithm Input: Constrained Priors		
Parameter	Value	
Data	CDF (Number of Infected)	
Distance Function	RMSE	
Max. No of Populations	12	
Population Size	1000	
Epsilon (ϵ)	Unspecified	
α	$\mathcal{U}(0.01, 0.05)$	
$eta_{ ext{Group 1}}$	${\cal U}(0.0, 0.4)$	
$eta_{ ext{Group 2}}$	\mathcal{U} (0.5, 0.8)	

Table B.5: pyABC ABC-SMC Algorithm Input: Homogeneous Configuration

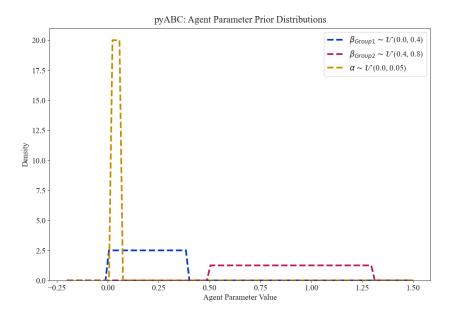


Figure B.6: pyABC Constrained Priors: Alpha and Beta Parameters are Uniformly Distributed

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

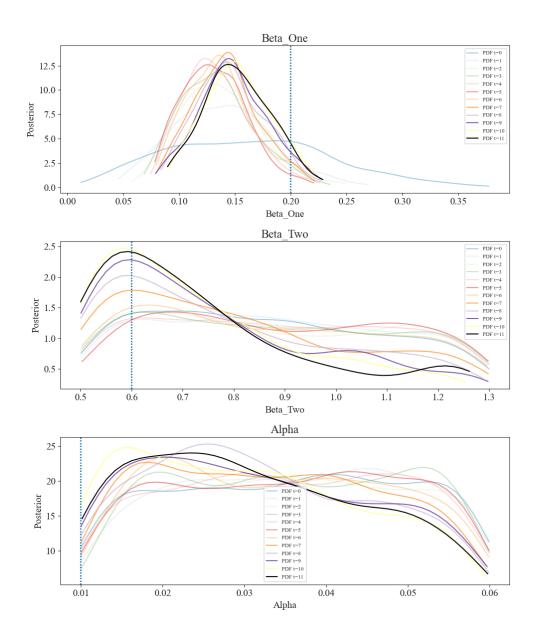


Figure B.7: pyABC Posteriors: Conditional Probability of Alpha and Beta Parameters

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

pyABC Algorithm Output: Posterior Modes			
No. of Donulations	Mode		
No. of Populations	α	$\beta_{ m Group \ 1}$	$\beta_{\text{Group 2}}$
0	0.04058033	0.19115846	0.69644518
1	0.0445686	0.14632727	0.82708123
2	0.0365159	0.12790874	0.61589995
3	0.05182846	0.1332135	0.63173797
4	0.0305015	0.12402448	0.61640069
5	0.04261005	0.12485908	0.68144975
6	0.02025336	0.13630381	0.63168193
7	0.01809786	0.14361261	0.59856792
8	0.02531923	0.14233784	0.59680371
9	0.0201772	0.14533129	0.5983028
10	0.01608586	0.1500786	0.57679122
11	0.02332019	0.14365612	0.5933509

Table B.6: pyABC Output: Posterior Mode of α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$

APPENDIX B. CHAPTER 5

B.3. APPROXIMATE BAYESIAN COMPUTATION EXERCISE: CON-STRAINED PRIORS

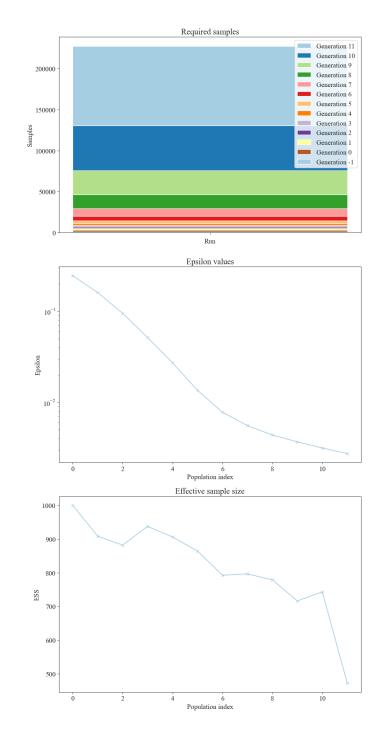


Figure B.8: pyABC Priors: Alpha and Beta Parameters are Uniformly Distributed

Appendix C

Chapter 6

C.1 PyABC: Heterogeneous Configuration of Alpha Parameters

This section contains the results of the pyABC exercise on the Heterogeneous Configuration of the case study ABM. Heterogeneity was expressed in α , rather than β .

pyABC ABC-SMC Algorithm Input		
Parameter	Value	
Data	CDF (Number of Infected)	
Distance Function	RMSE	
Max. No of Populations	12	
Population Size	1000	
Epsilon (ϵ)	Unspecified	
β	U(0.0, 0.1)	
$\alpha_{ m Group 1}$	U(0.0, 1.0)	
$\alpha_{ m Group 2}$	${\cal U}$ (0.0, 1.0)	

Table C.1: pyABC ABC-SMC Algorithm Input: Heterogeneous Configuration

C.1. PYABC: HETEROGENEOUS CONFIGURATION OF ALPHA PARAMETERS

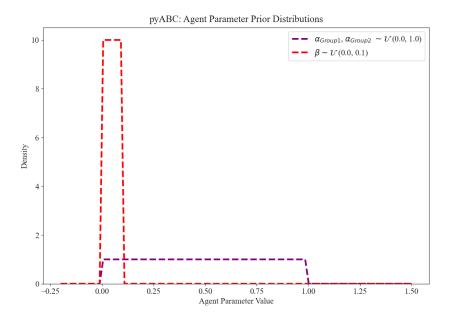


Figure C.1: pyABC Priors: Alpha and Beta Parameters are Uniformly Distributed

C.1. PYABC: HETEROGENEOUS CONFIGURATION OF ALPHA PARAMETERS

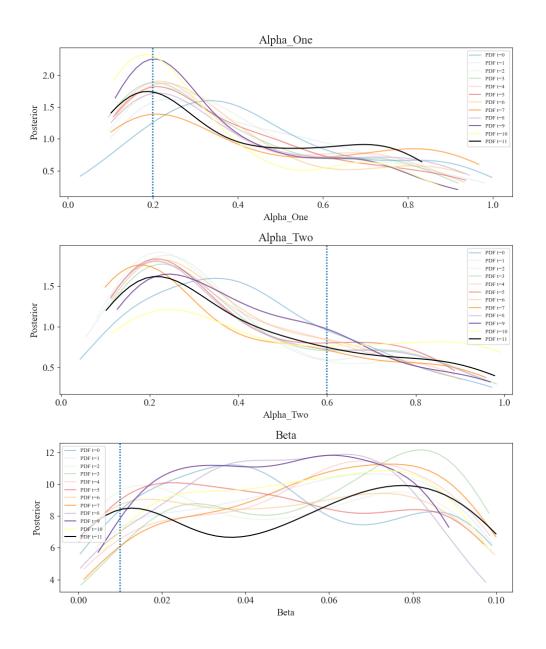


Figure C.2: pyABC Posteriors: Conditional Probability of Alpha

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C.1. PYABC: HETEROGENEOUS CONFIGURATION OF ALPHA PARAMETERS

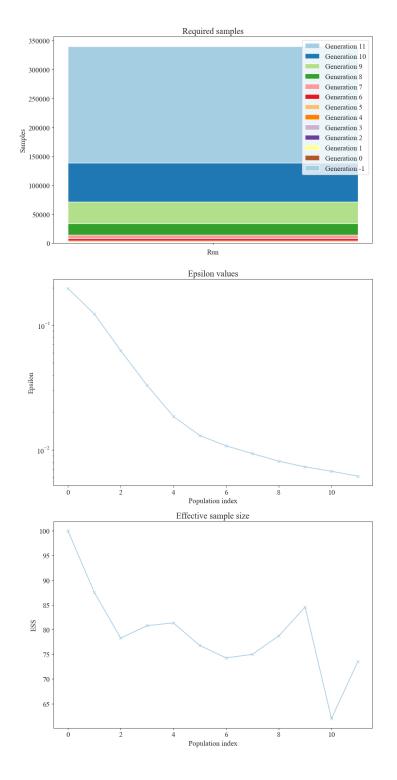


Figure C.3: pyABC Output: Conditional Probability of Alpha

pyABC Algorithm Output: Posterior Modes			
Mode			
eta	$\alpha_{ m Group 1}$	$\alpha_{ m Group 2}$	
0.03660193	0.32527573	0.34632693	
0.06994286	0.2435832	0.24325429	
0.0147038	0.23212959	0.21397648	
0.08230054	0.19566246	0.2358787	
0.06880536	0.21258378	0.20694185	
0.02181635	0.20824475	0.22295073	
0.07319986	0.230185	0.22739194	
0.0737856	0.206936	0.18706675	
0.06382852	0.20486102	0.21697969	
0.06126214	0.20990235	0.24698206	
0.07378815	0.18564859	0.2395132	
0.07763232	0.19090389	0.20896333	
	β 0.03660193 0.06994286 0.0147038 0.08230054 0.06880536 0.02181635 0.07319986 0.0737856 0.06382852 0.06126214 0.07378815	Mode β αGroup 1 0.03660193 0.32527573 0.06994286 0.2435832 0.0147038 0.23212959 0.08230054 0.19566246 0.06880536 0.21258378 0.02181635 0.20824475 0.07319986 0.230185 0.06382852 0.20486102 0.06126214 0.20990235 0.07378815 0.18564859	

Table C.2: pyABC Output: Posterior Mode of β , $\alpha_{\text{Group 1}}$ and $\alpha_{\text{Group 2}}$

C.2 PyABC: Varying Beta Parameters

This section presents the results of pyABC analysis on the Heterogeneous Configuration of the case study ABM, where the β parameters are numerically closer.

Heterogeneous Config: ABM Parameters		
Parameter	Value	
Number of Agents	1000	
Number of Iterations (Time, t)	1000	
Single Instance	1(t)	
Number of Agent Groups	2	
α	0.01	
$eta_{ ext{Group 1}}$	0.5	
$eta_{ ext{Group 2}}$	0.6	
γ	0.1	
α $\beta_{\text{Group 1}}$	2 0.01 0.5 0.6	

Table C.3: Heterogeneous Configuration Parameter Values: Observed Data

C.2. PYABC: VARYING BETA PARAMETERS

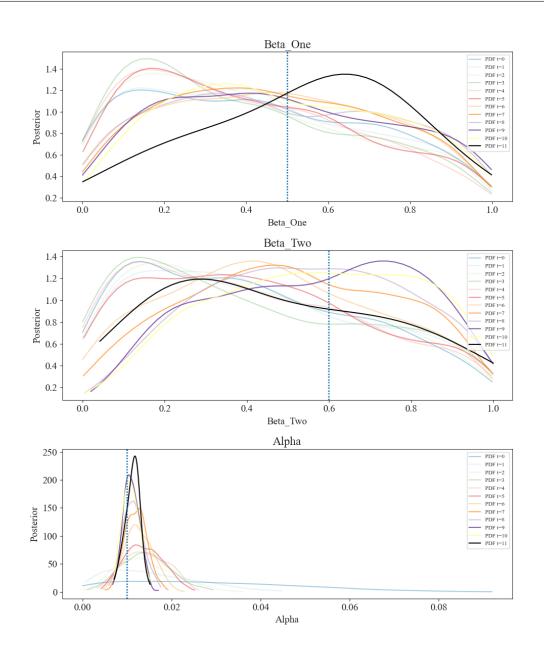


Figure C.4: pyABC Posteriors: Conditional Probability of Beta

APPENDIX C. CHAPTER 6

C.2. PYABC: VARYING BETA PARAMETERS

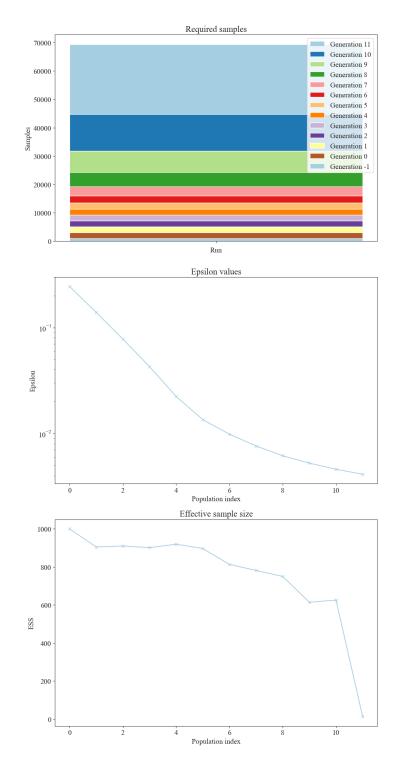


Figure C.5: pyABC Output: Conditional Probability of Alpha

pyABC Algorithm Output: Posterior Modes			
No. of Populations	Mode		
No. of Populations	α	$\beta_{ ext{Group 1}}$	$\beta_{ m Group \ 2}$
0	0.01128307	0.14378275	0.14259804
1	0.00777791	0.14270492	0.18310219
2	0.01255396	0.18349323	0.18344775
3	0.01378332	0.16319265	0.14309561
4	0.01254974	0.16510232	0.1422163
5	0.01188563	0.16462569	0.34549207
6	0.01162137	0.46900349	0.40747905
7	0.01285864	0.38665268	0.46991308
8	0.0114102	0.32709762	0.47142065
9	0.01034748	0.40785543	0.73983918
10	0.01060047	0.34838488	0.57239132
11	0.01171806	0.63207576	0.29613587

Table C.4: pyABC Output: Posterior Mode of α , $\beta_{\text{Group 1}}$ and $\beta_{\text{Group 2}}$

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